Finding High-Quality Local Minima in Derivative-Free Optimization

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Motivation

- We want to identify distinct, “high-quality”, local minimizers of

$$\begin{aligned} \text{minimize } & f(x) \\ l \leq x & \leq u \\ x & \in \mathbb{R}^n \end{aligned}$$

- High-quality can be measured by more than the objective.

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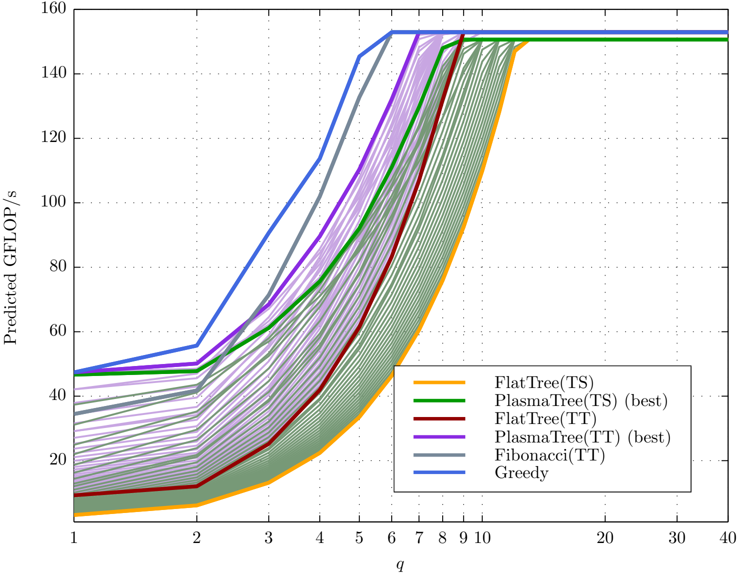
- Derivatives of f may or may not be available.
- The simulation f is likely using parallel resources, but it does not utilize the entire machine.

Why concurrency? Tiled QR example



[Bouwmeester, et al., Tiled QR Factorization Algorithms, 2011]

Global optimization is difficult

Theorem (Törn and Žilinskas, *Global Optimization*, 1989)

An algorithm converges to the global minimum of any continuous f on a domain $\mathcal{D}$ if and only if the algorithm generates iterates that are dense in $\mathcal{D}$.

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  - convex f
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  - finite domain $\mathcal{D}$

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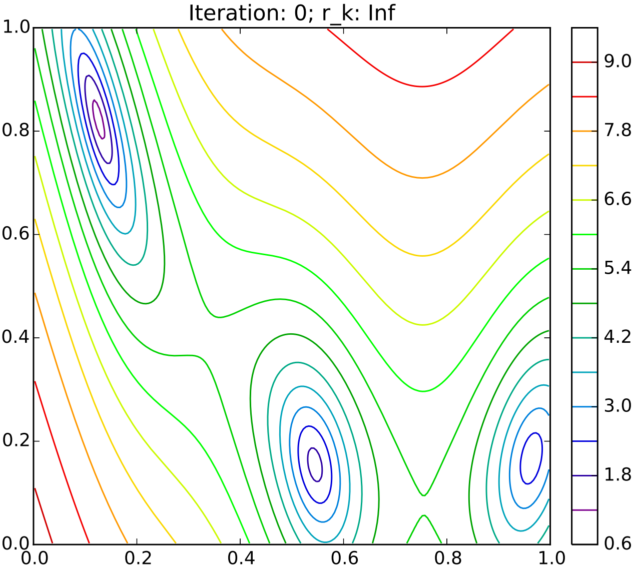
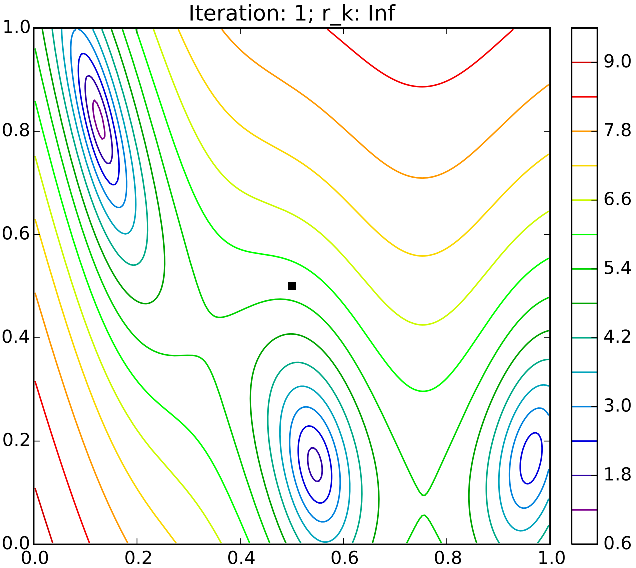
An algorithm must trade-off between "refinement" and "exploration".

DIRECT

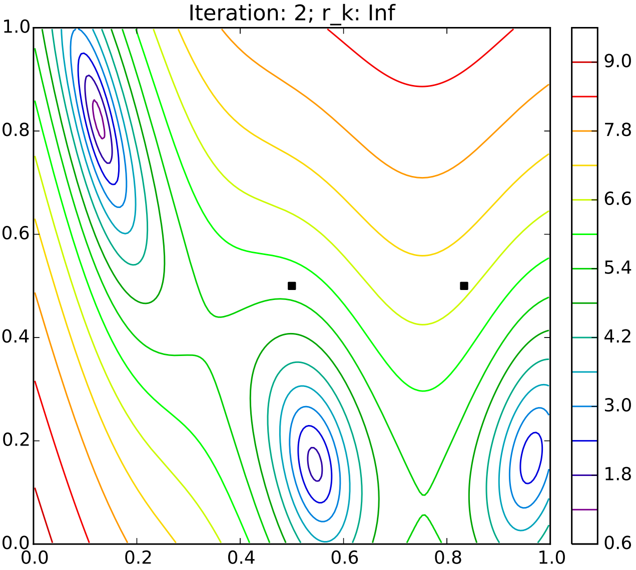

Iteration: 0; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



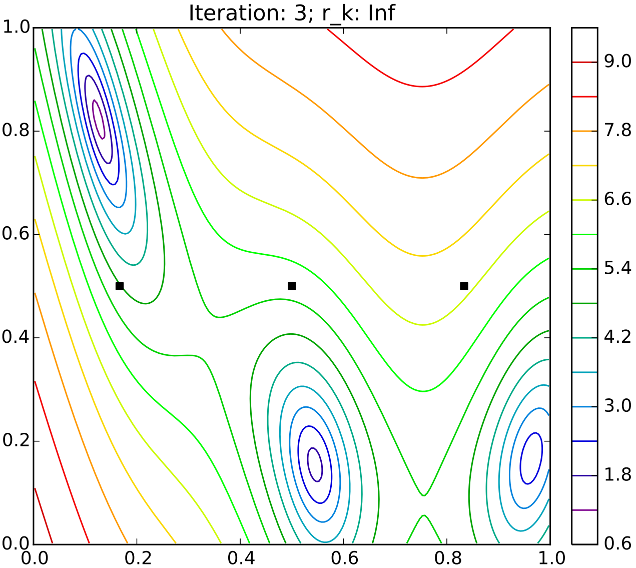
Iteration: 1; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



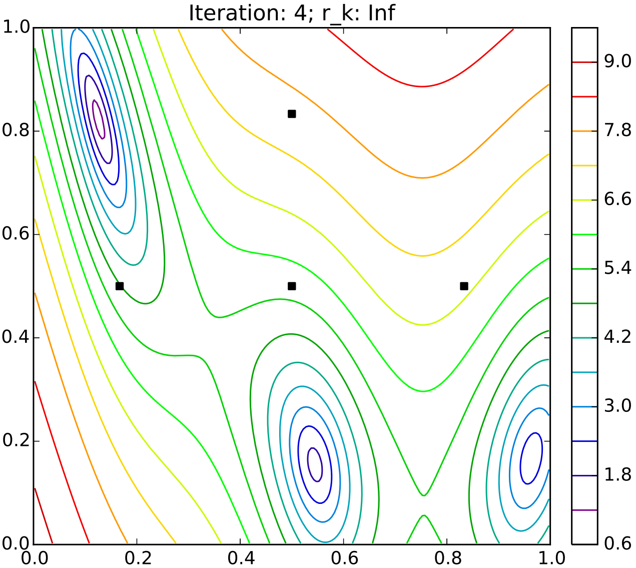
Iteration: 2; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



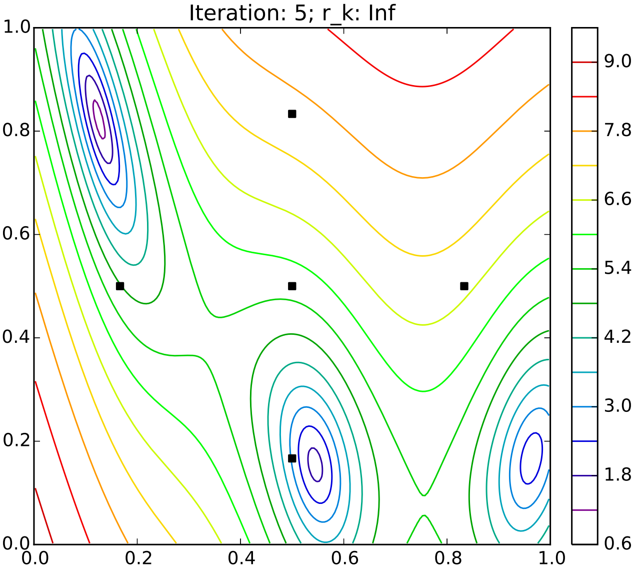
Iteration: 3; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



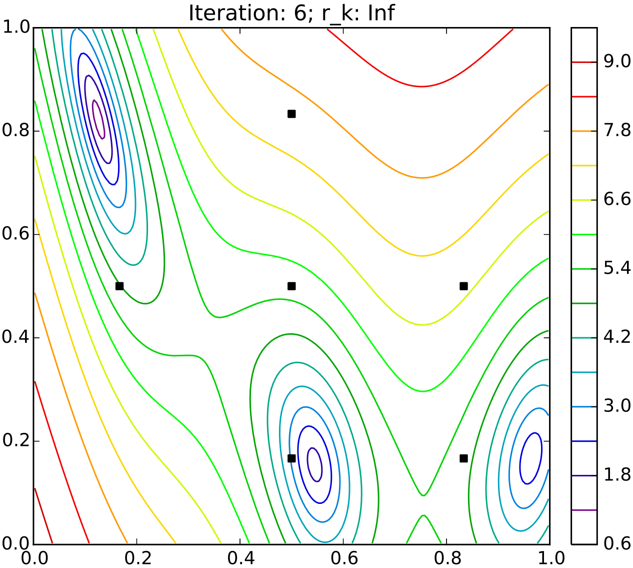
Iteration: 4; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



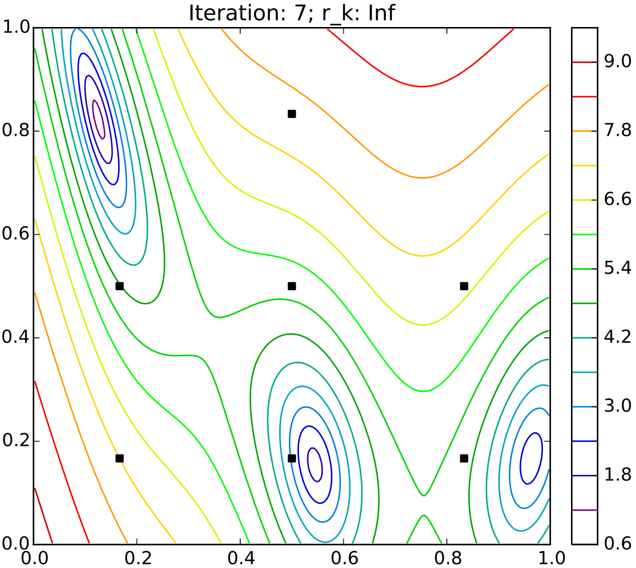
Iteration: 5; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



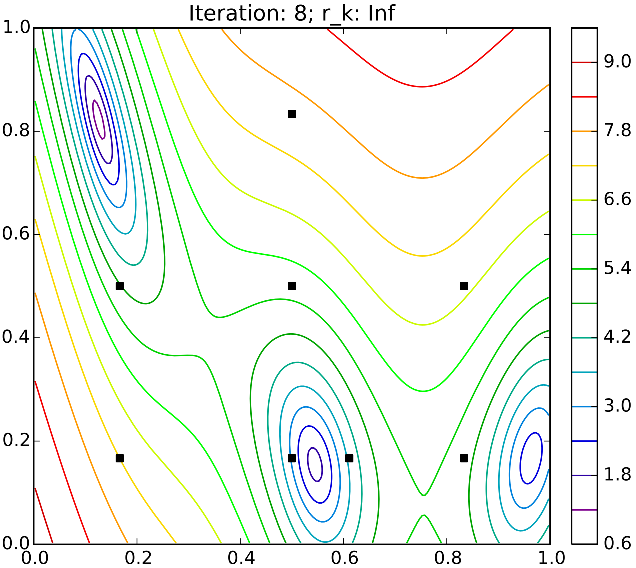
Iteration: 6; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



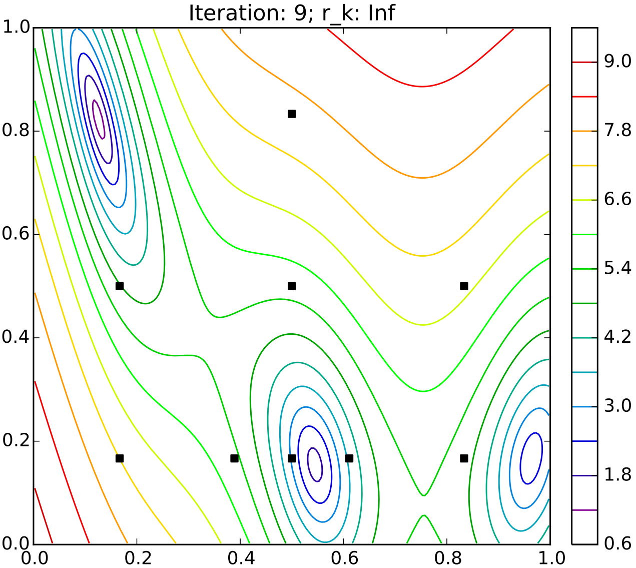
Iteration: 7; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



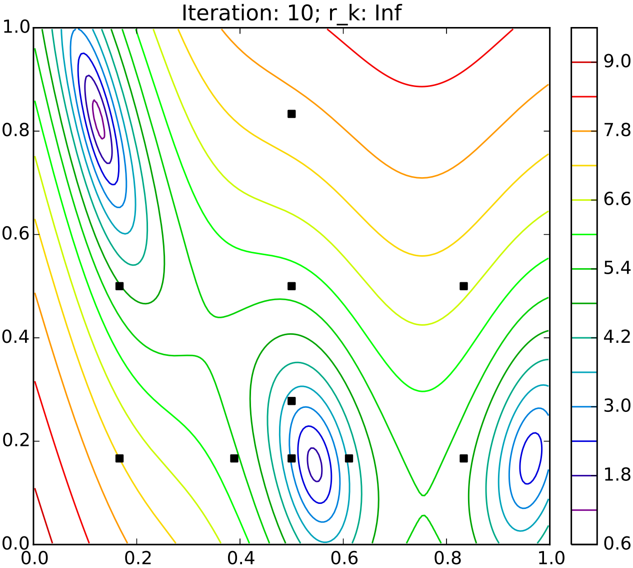
Iteration: 8; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



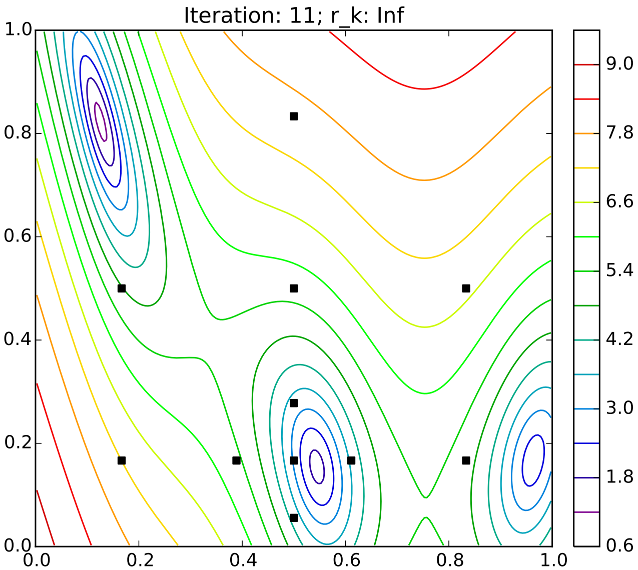
Iteration: 9; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



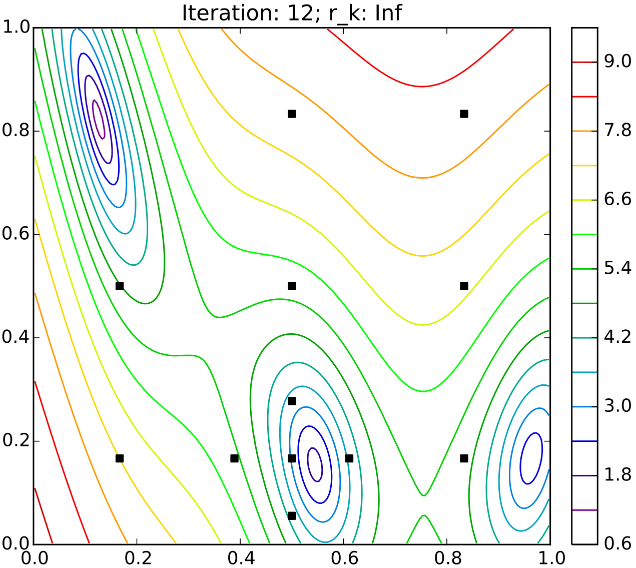
Iteration: 10; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



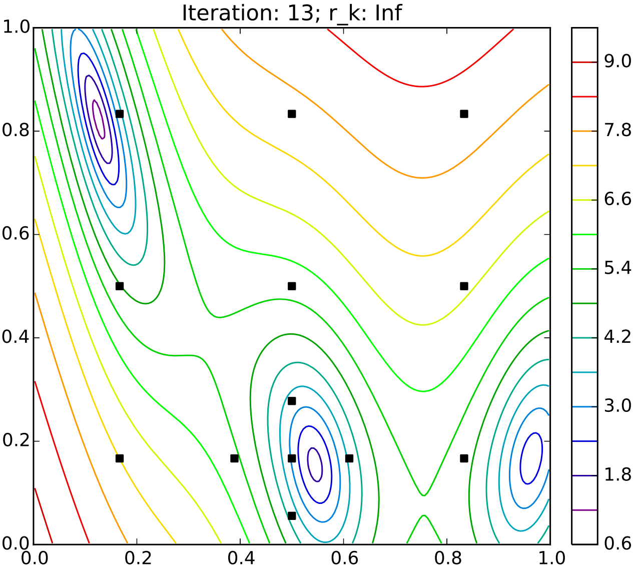
Iteration: 11; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



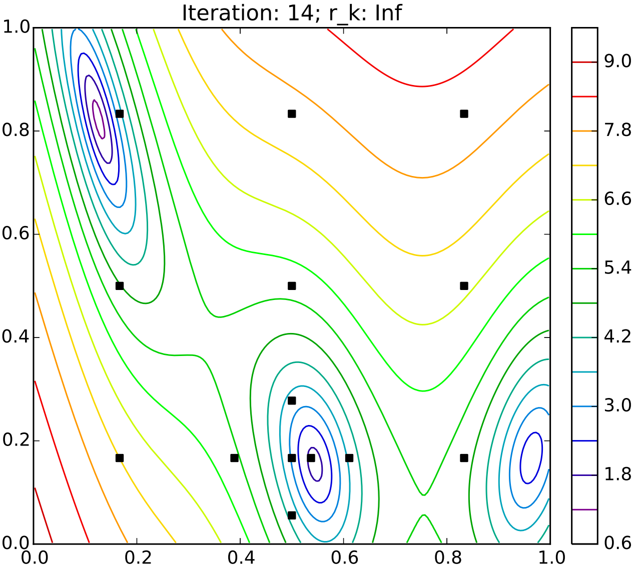
Iteration: 12; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



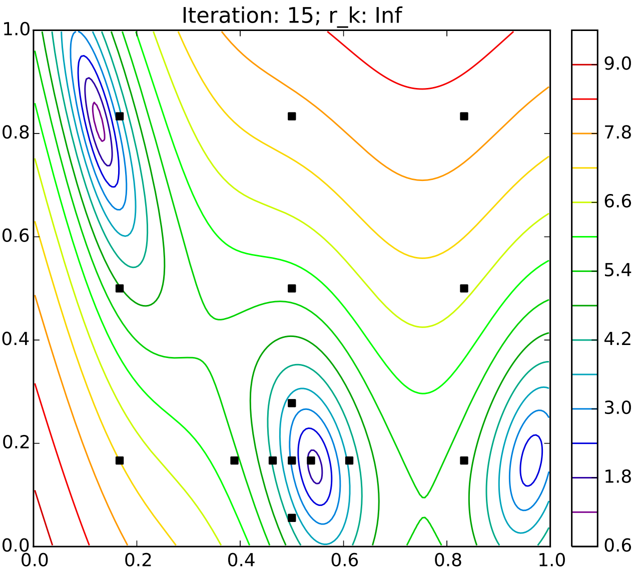
Iteration: 13; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



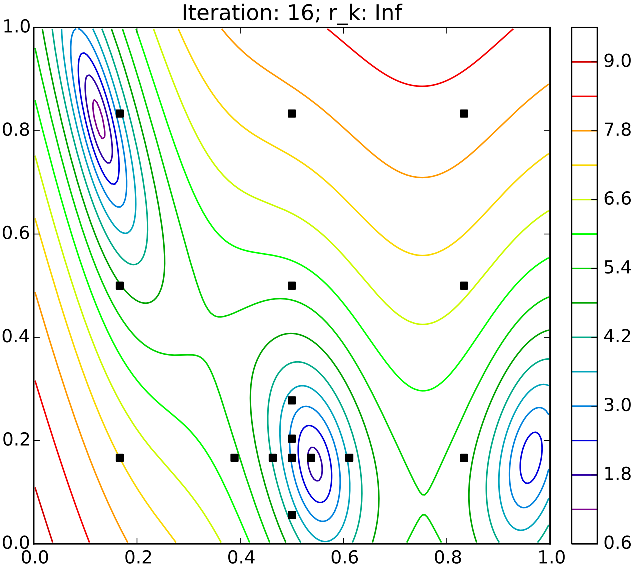
Iteration: 14; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



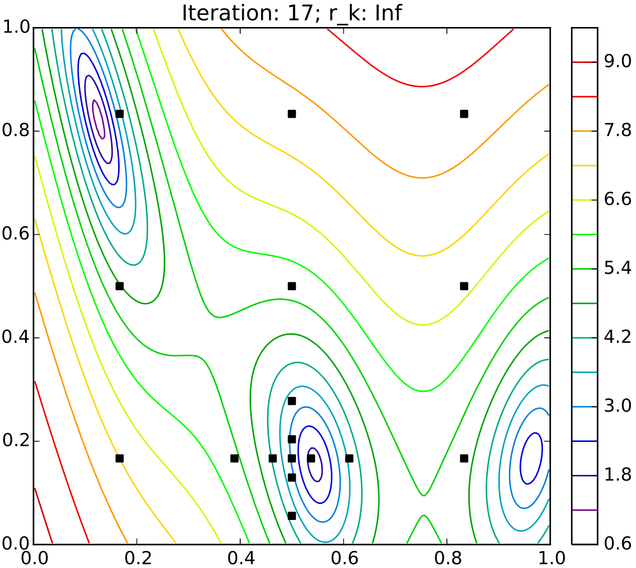
Iteration: 15; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



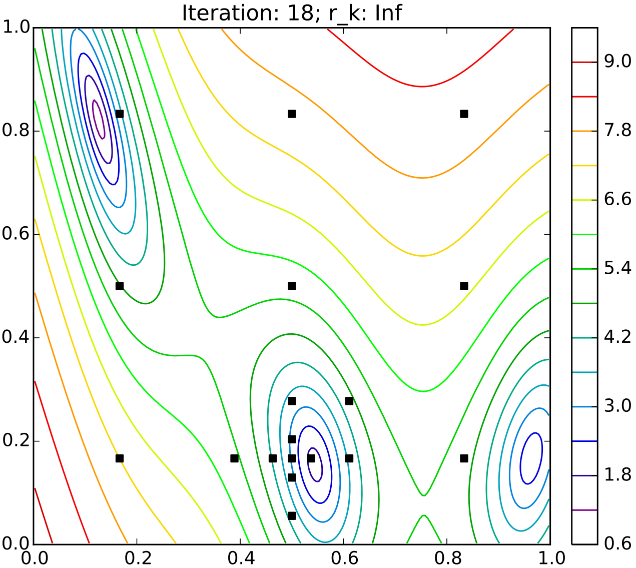
Iteration: 16; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



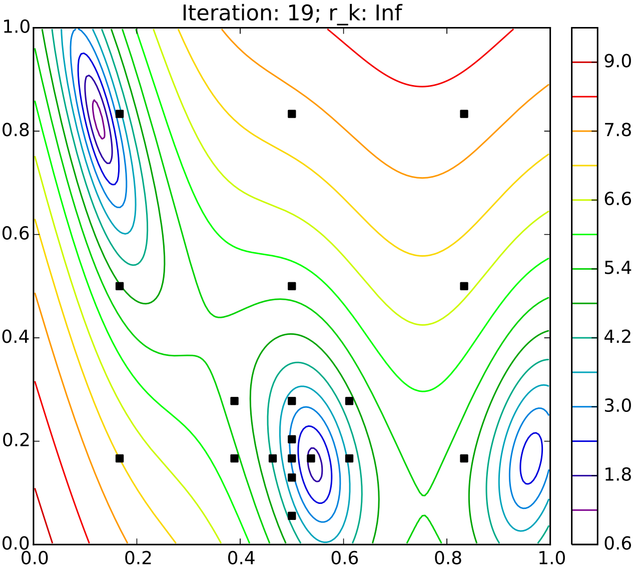
Iteration: 17; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



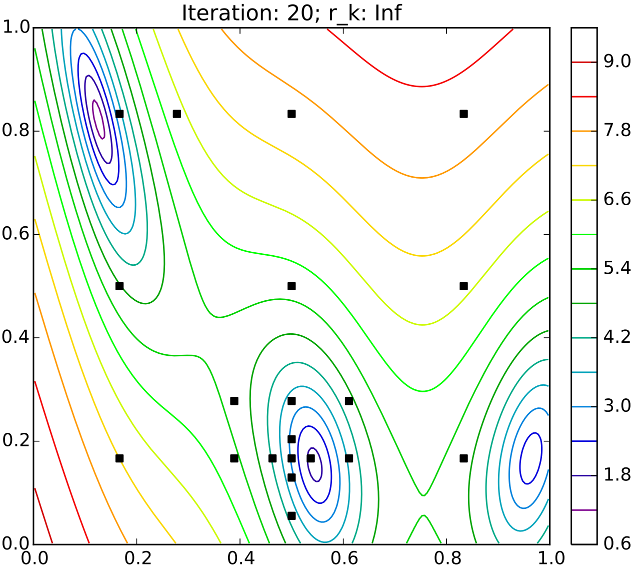
Iteration: 18; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



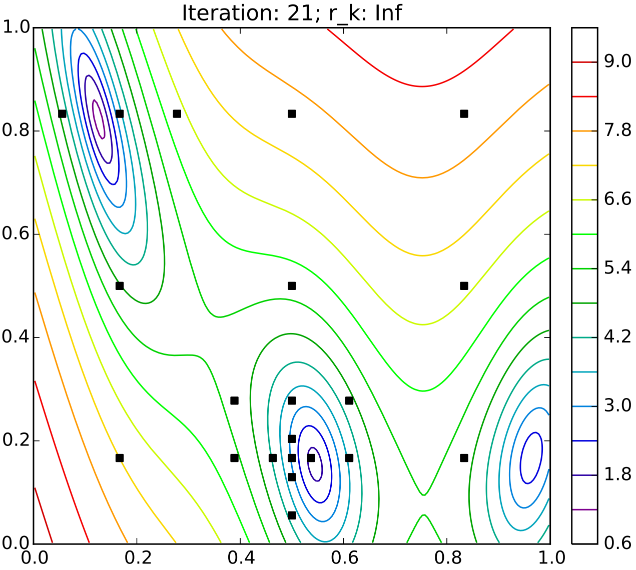
Iteration: 19; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



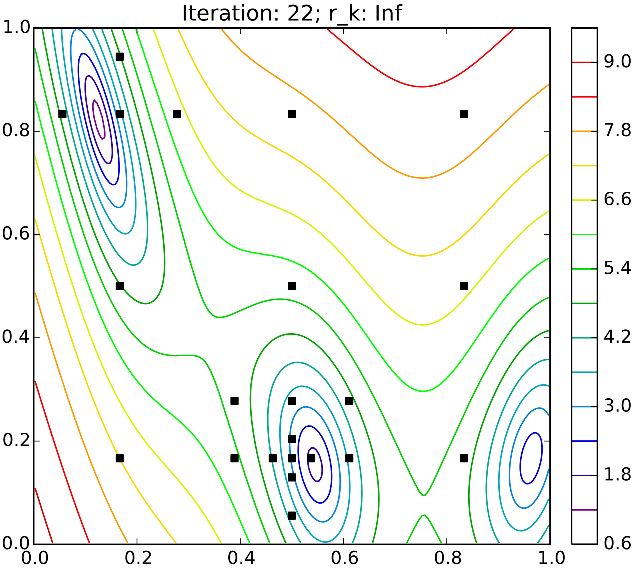
Iteration: 20; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



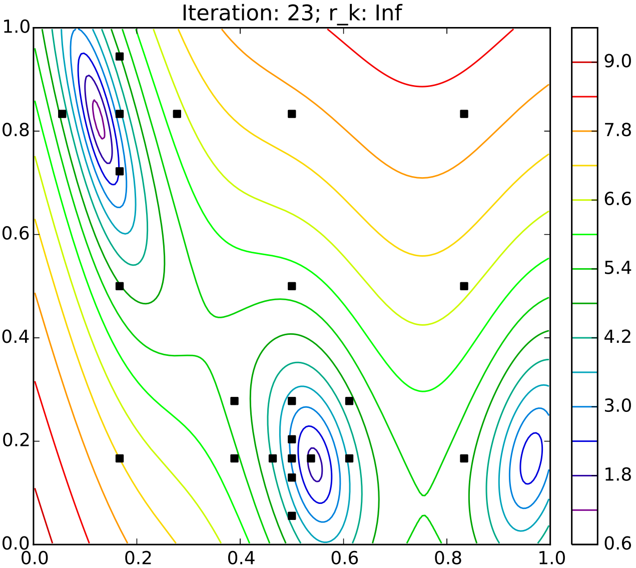
Iteration: 21; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT

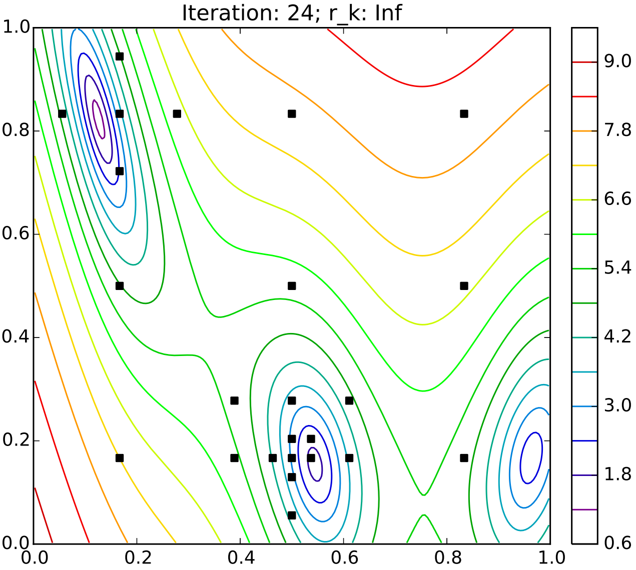


Iteration: 22; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT

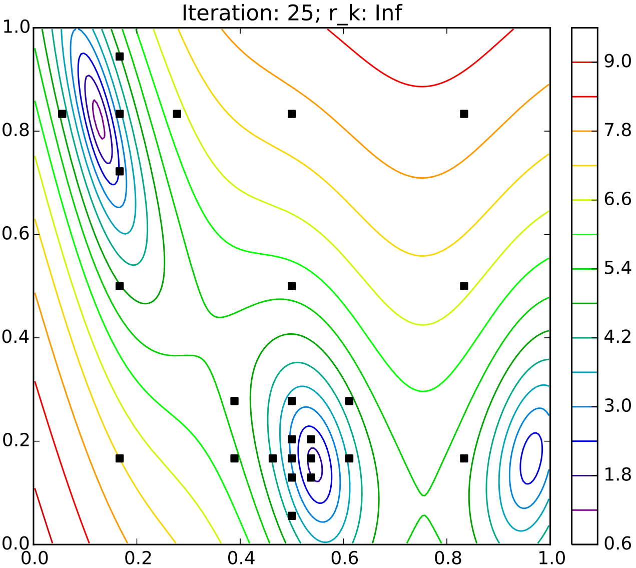

Iteration: 23; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



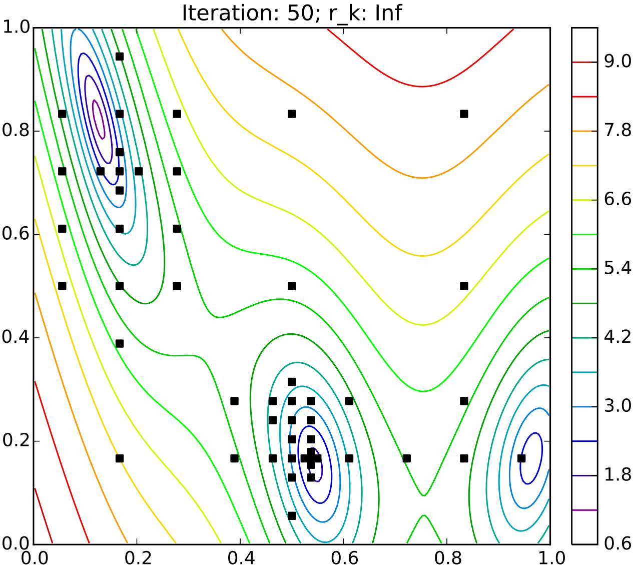
Iteration: 24; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT

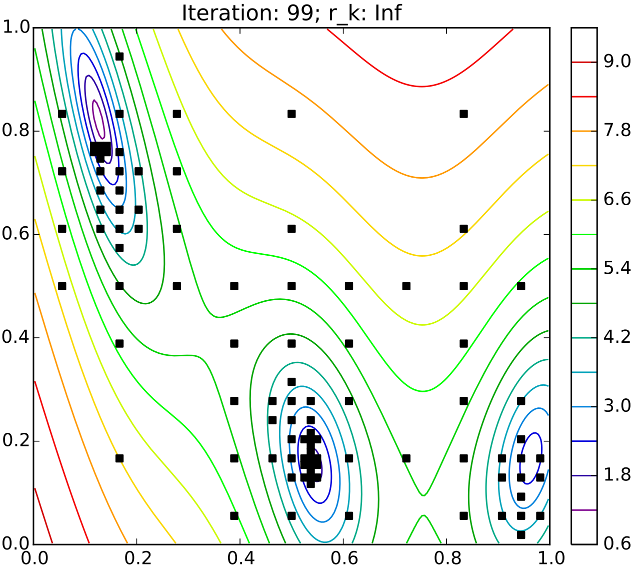


Iteration: 25; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT

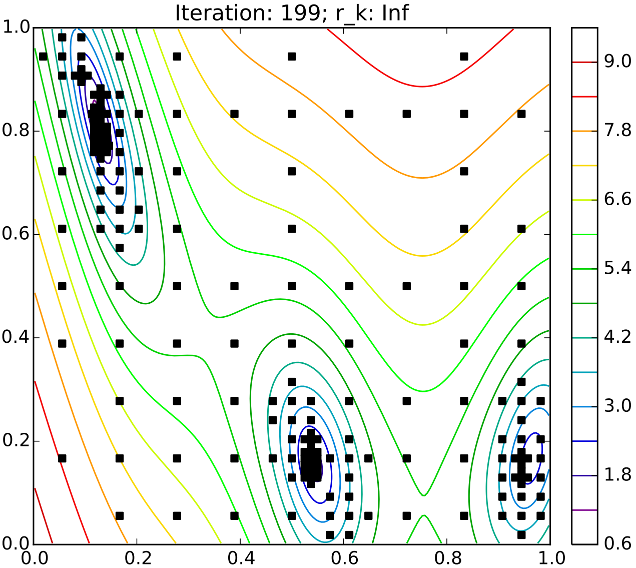

Iteration: 50; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



Iteration: 99; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

DIRECT



Iteration: 199; r_k: Inf
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
9.0
7.8
6.6
5.4
4.2
3.0
1.8
0.6

Multistart Methods

Given some local optimization routine L:

Algorithm 1: General Multistart

for $k = 1, 2, \ldots$ **do**

  Evaluate f at N points drawn from $\mathcal{D}$

  Start L at some set (possibly empty) of previously evaluated points

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- Get to use problem specific local optimization routines.
- Possibly multiple levels of parallelism (objective, local method, global method); L may involve many sequential evaluations of f...

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- If resources are limited, how should points from each run receive priority?

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- If resources are limited, how should points from each run receive priority?

- Ideally, only one run is started for each minima.
- Exploring by sampling. Refining with L.

Multi-Level Single Linkage

Given some local optimization routine L:

Algorithm 2: MLSL

for $k = 1, 2, \dots$ **do**

Sample f at N random points drawn uniformly from $\mathcal{D}$

Start L at all sample points x:

- that has yet to start a run
- $\nexists x_i : \|x - x_i\| \leq r_k$ and $f(x_i) < f(x)$

[Rinnooy Kan and Timmer, *Mathematical Programming*, 39(1):57–78, 1987]

Multi-Level Single Linkage

Given some local optimization routine L:

Algorithm 2: MLSL

for $k = 1, 2, \ldots$ **do**

Sample f at N random points drawn uniformly from $\mathcal{D}$

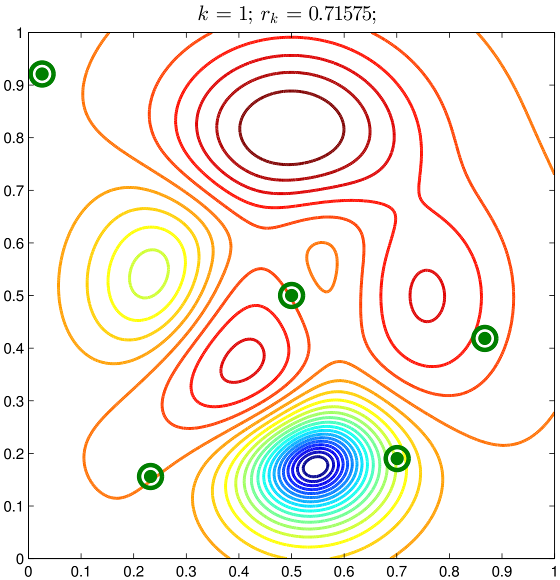
Start L at all sample points x:

- that has yet to start a run
- $\nexists x_i : \|x - x_i\| \leq r_k$ and $f(x_i) < f(x)$

[Rinnooy Kan and Timmer, *Mathematical Programming*, 39(1):57–78, 1987]

- Doesn't naturally translate when evaluations of f are limited
- Ignores some points when deciding where to start L

Multi-Level Single Linkage



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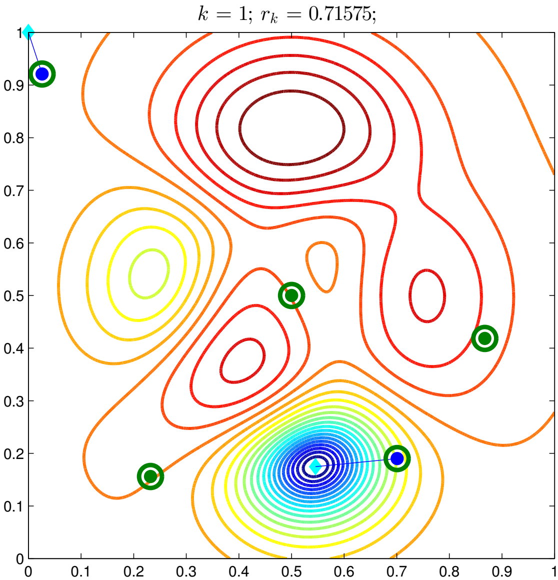

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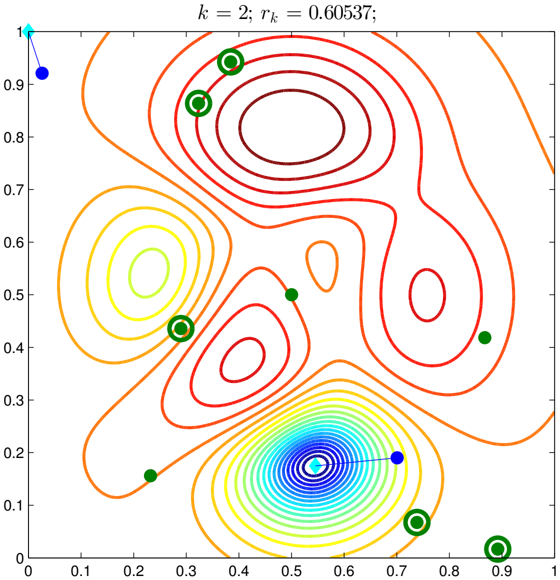

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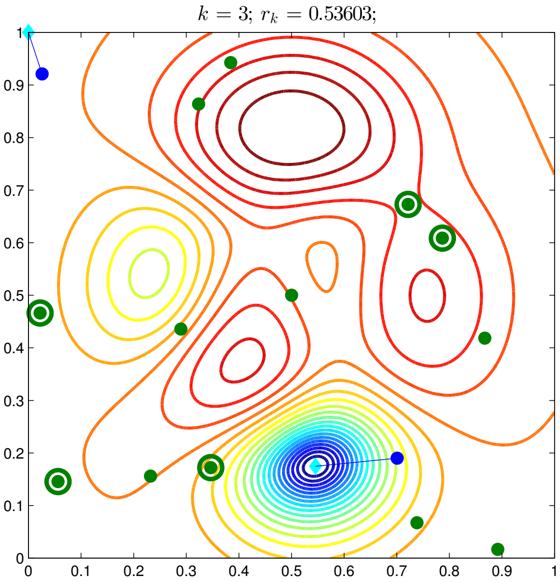

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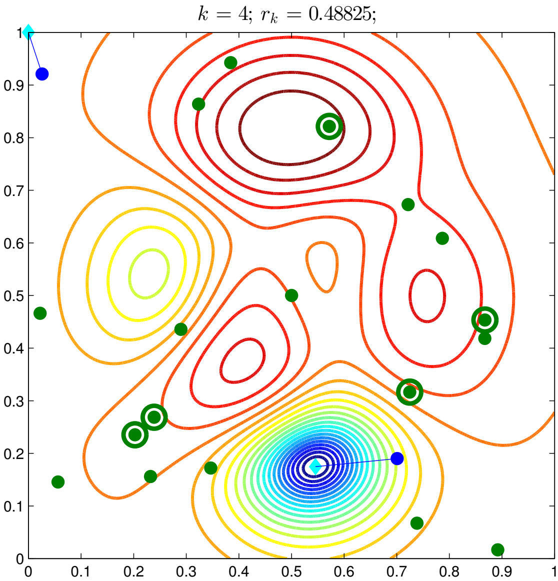

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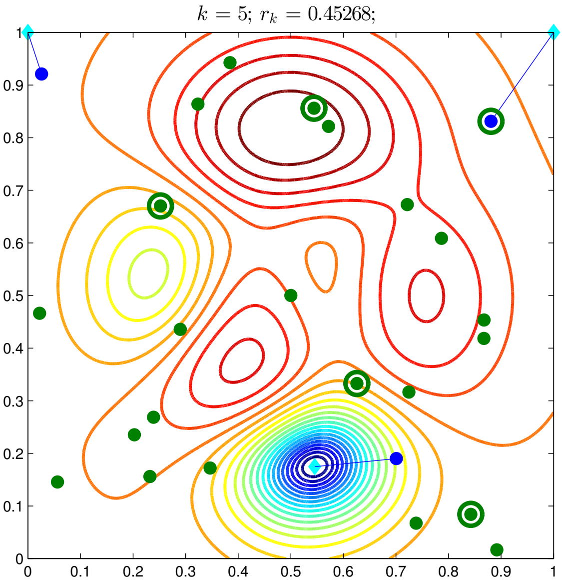

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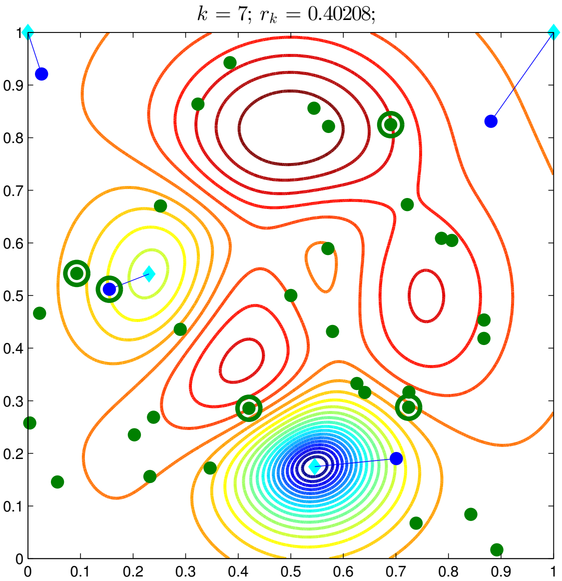

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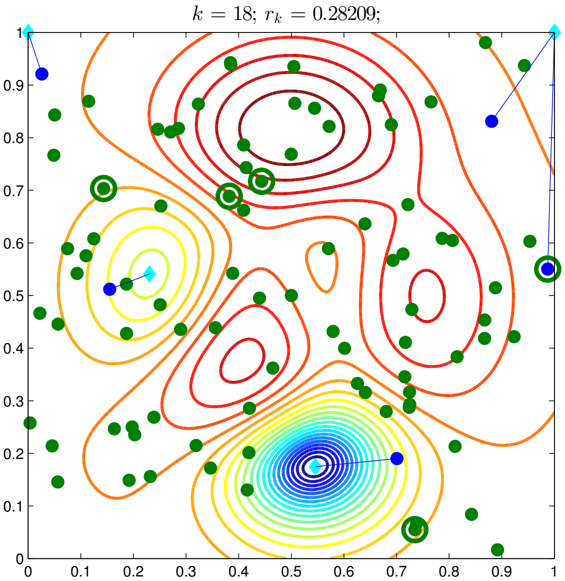

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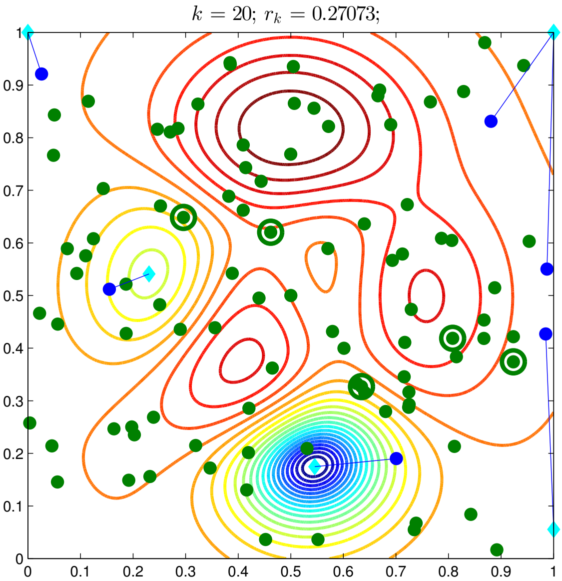

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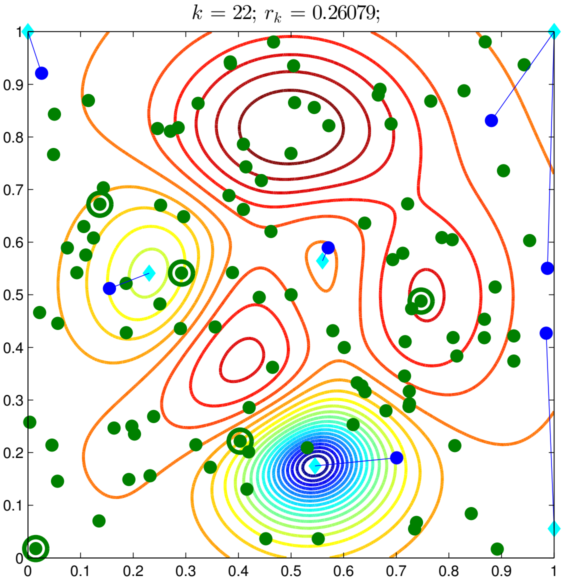

Multi-Level Single Linkage

- $f \in C^1$, with local minima in the interior of $\mathcal{D}$, and the distance between these minima is bounded away from zero.
- L is strictly descent and converges to a minimum (not a stationary point).
- $$r_k = \frac{1}{\sqrt{\pi}} \sqrt[n]{\Gamma\left(1 + \frac{n}{2}\right) \mathrm{vol}\left(\mathcal{D}\right) \frac{\sigma \log kN}{kN}} \qquad (1)$$

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Theorem

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Theorem

If $r_k \to 0$, all local minima will be found almost surely.

If r_k is defined by (1) with $\sigma > 4$, even if the sampling continues forever, the total number of local searches started is finite almost surely.

POSMM

MLSL: (S2)–(S4)

$\hat{x} \in S_k$

(S2) $\nexists x \in S_k$ *with*
$[\|\hat{x} - x\| \leq r_k$ *and* $f(x) < f(\hat{x})]$

(S3) $\hat{x}$ *has not started a local optimization run*

(S4) $\hat{x}$ *is at least* μ *from* $\partial\mathcal{D}$ *and* ν *from known local minima*

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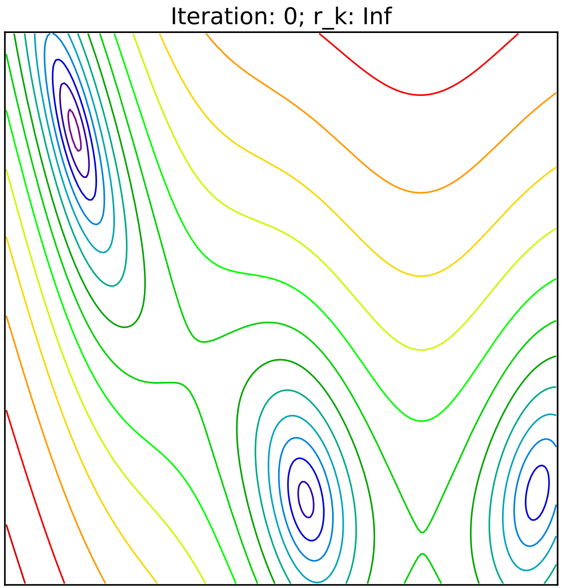
(L5) $\hat{x}$ is not in an active local optimization run and has not been ruled stationary

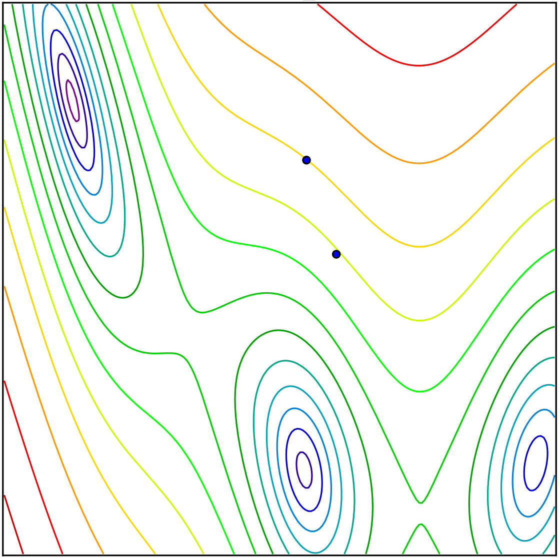
(L6) $\exists r_k$-descent path in H_k from some $x \in S_k$ satisfying (S2-S4) to $\hat{x}$

POSMM

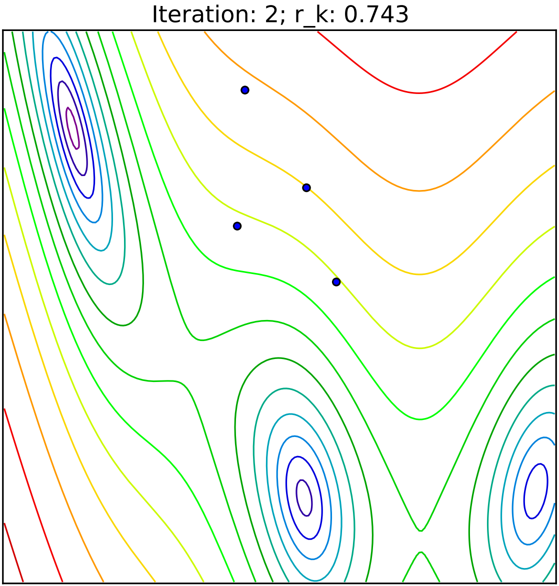


POSMM

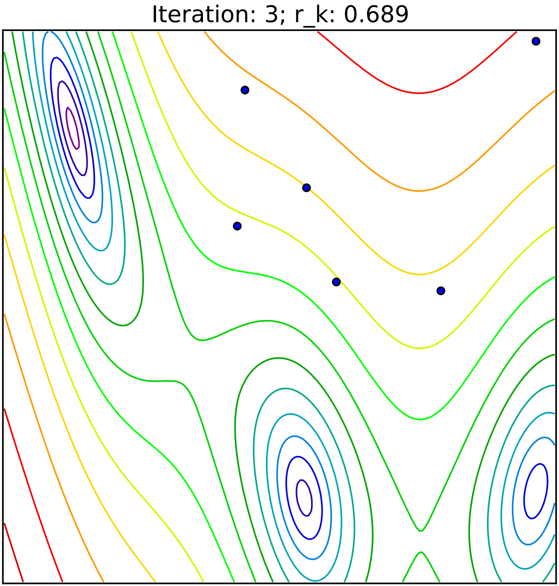
Iteration: 1; r_k: 0.743



POSMM



POSMM



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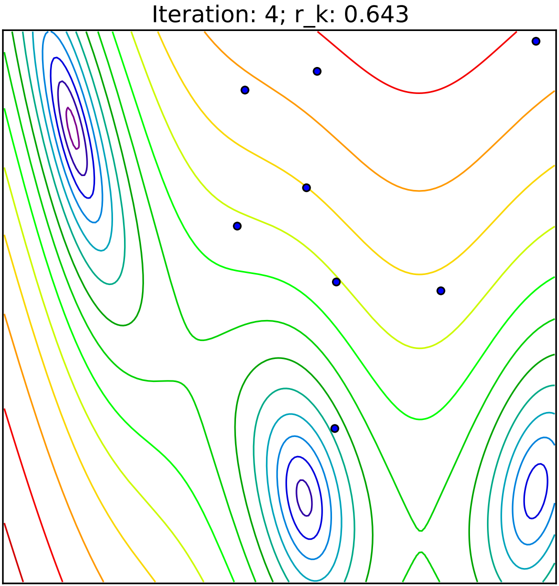

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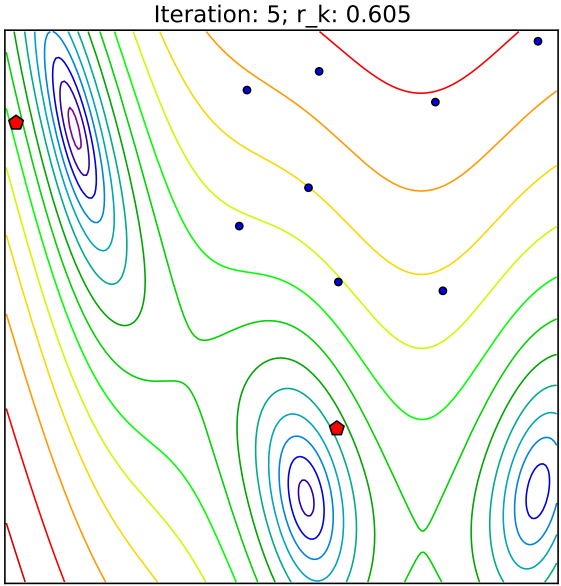

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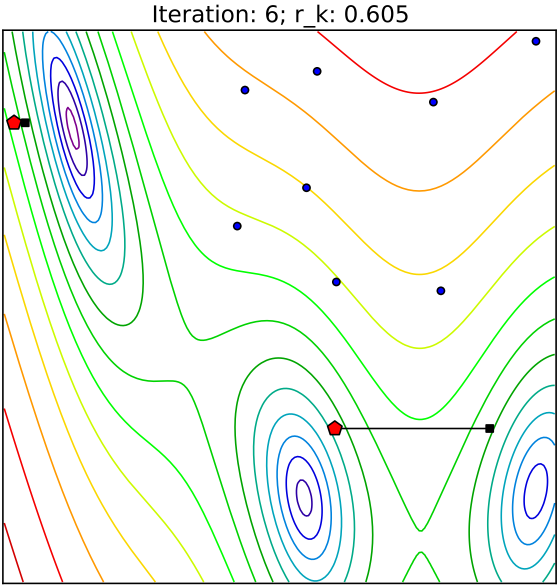

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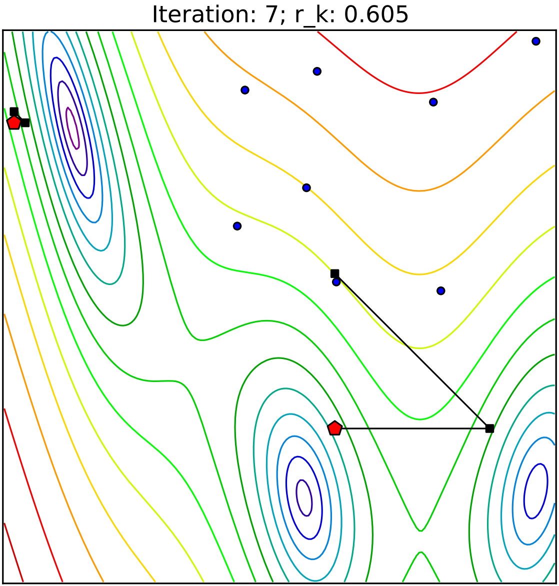

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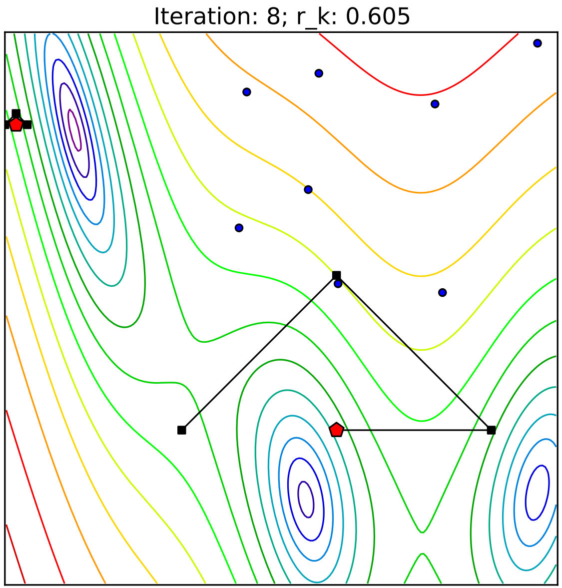

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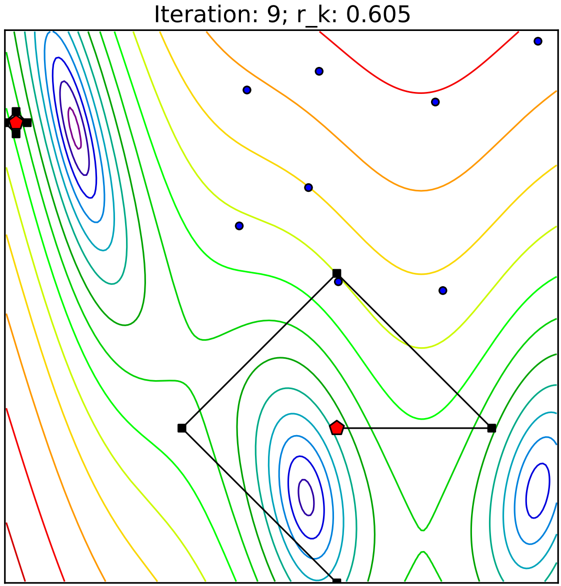

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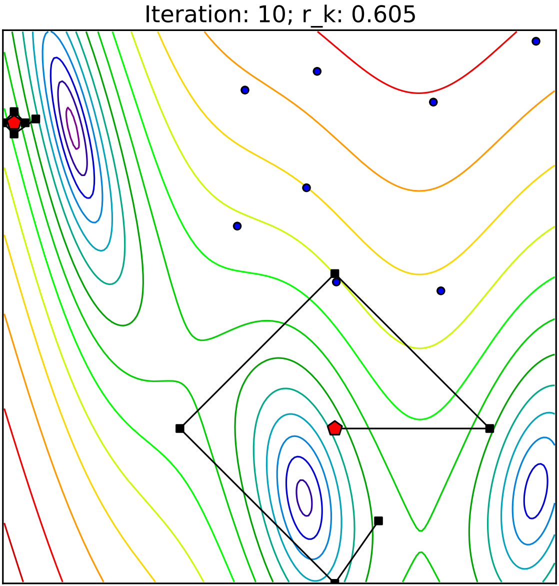

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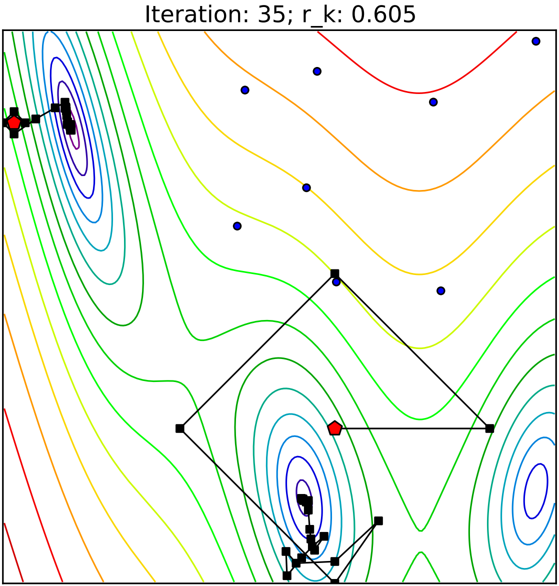

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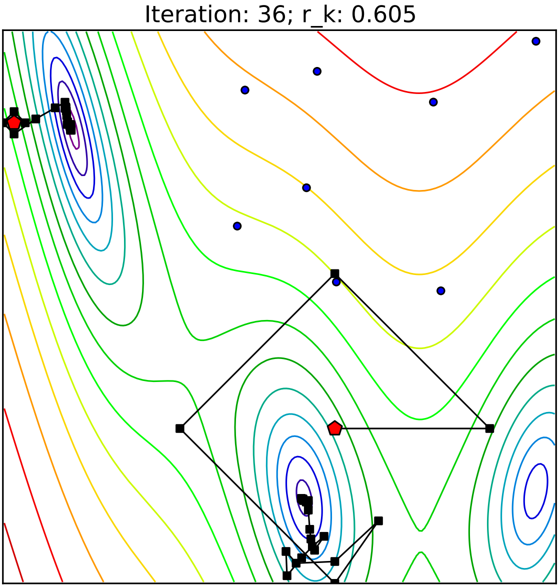

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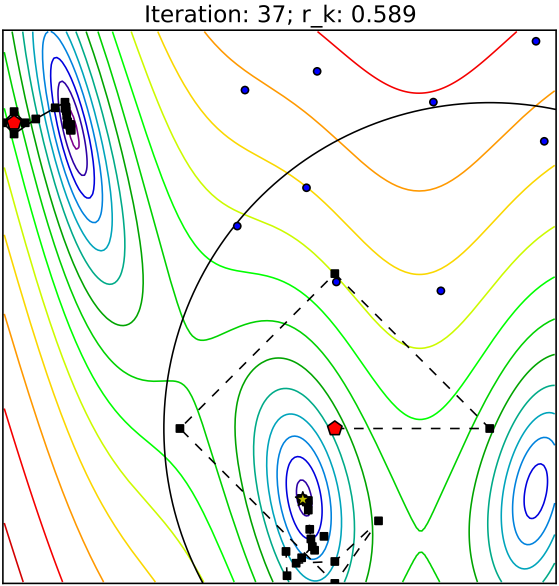

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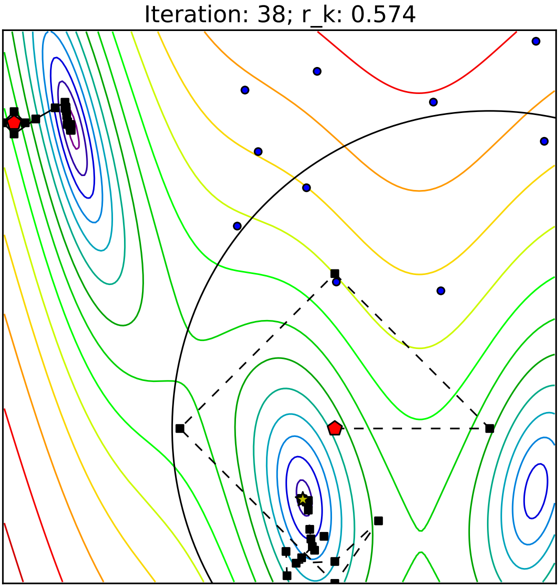

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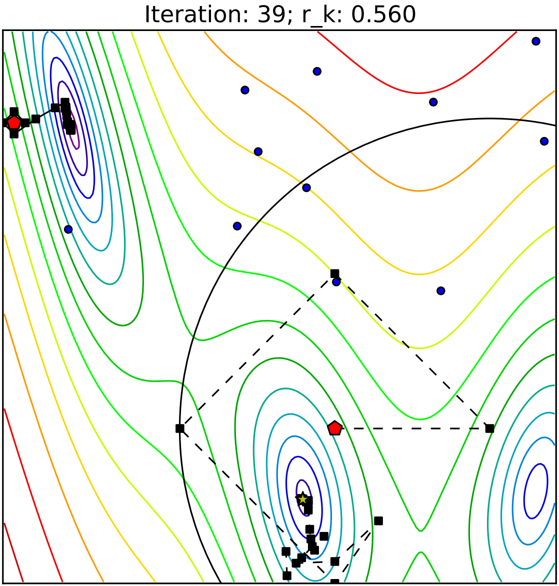

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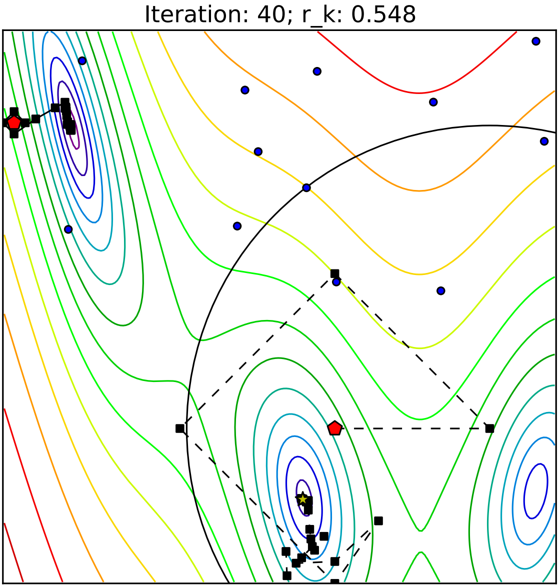

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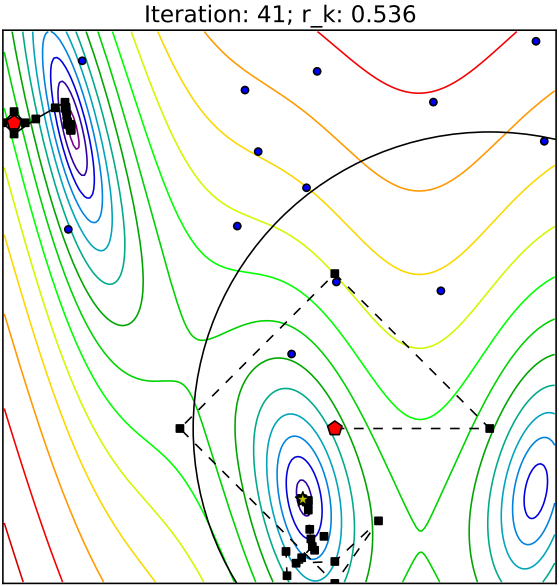

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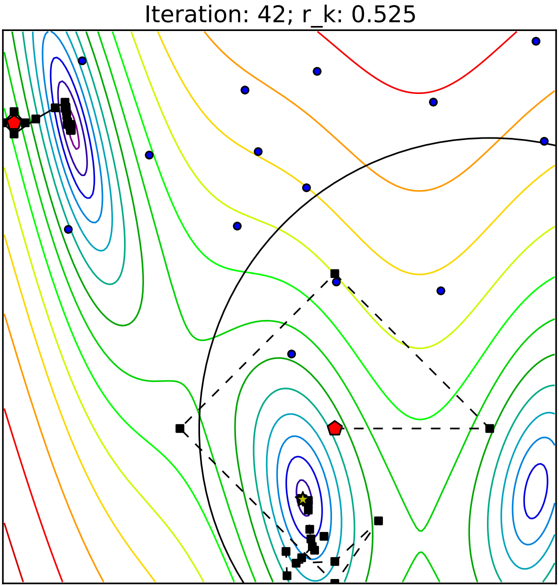

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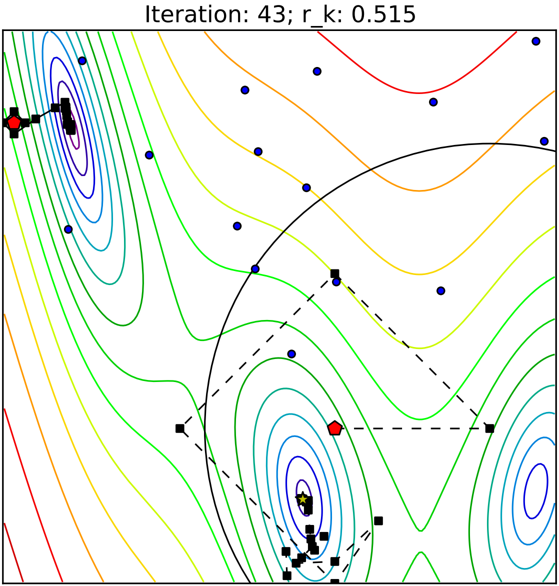

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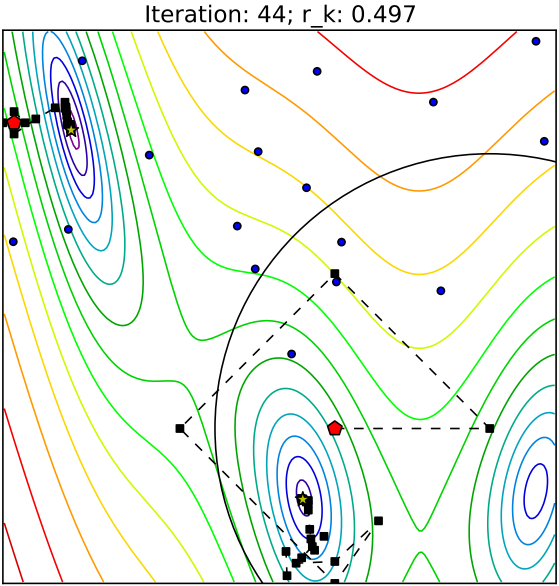

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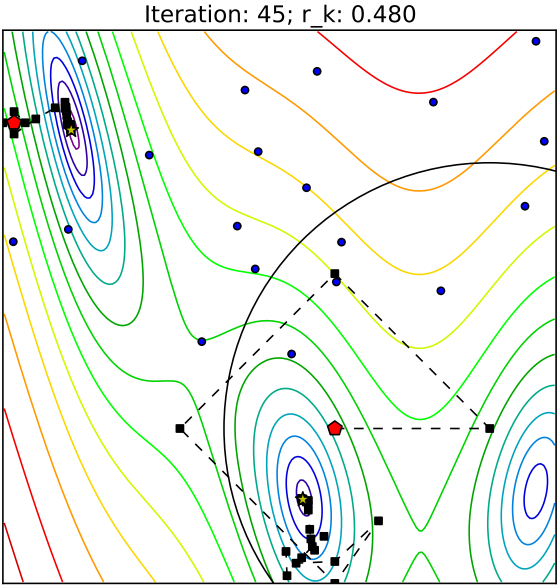
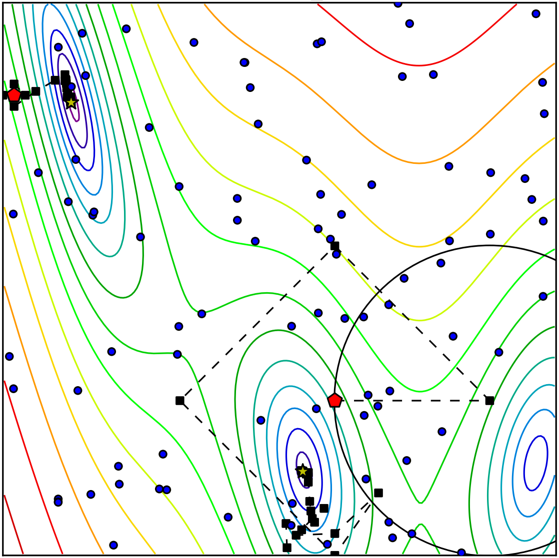


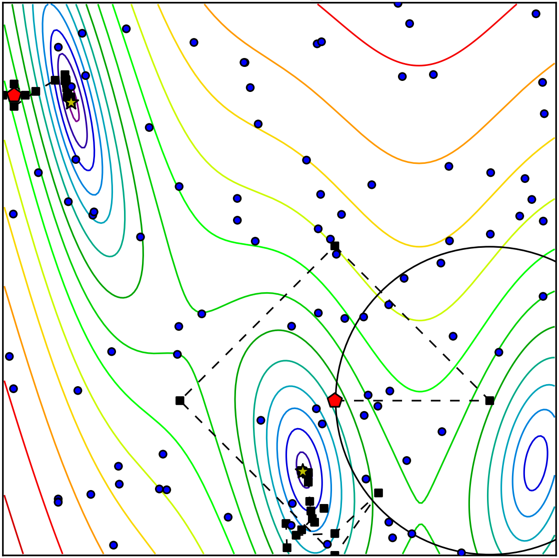
POSMM

Iteration: 80; r_k: 0.281



POSMM

Iteration: 81; r_k: 0.279



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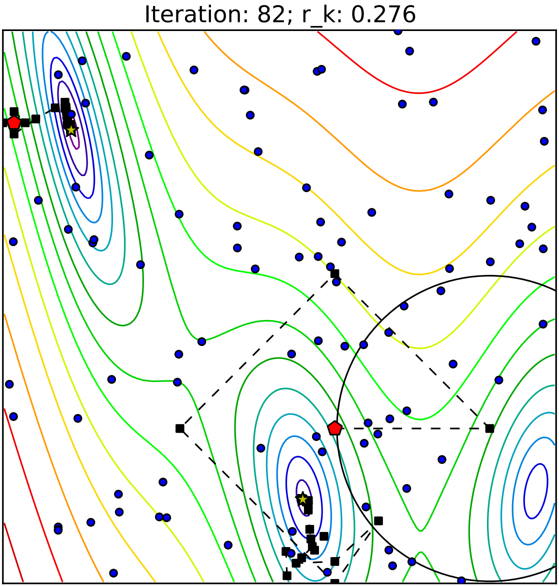

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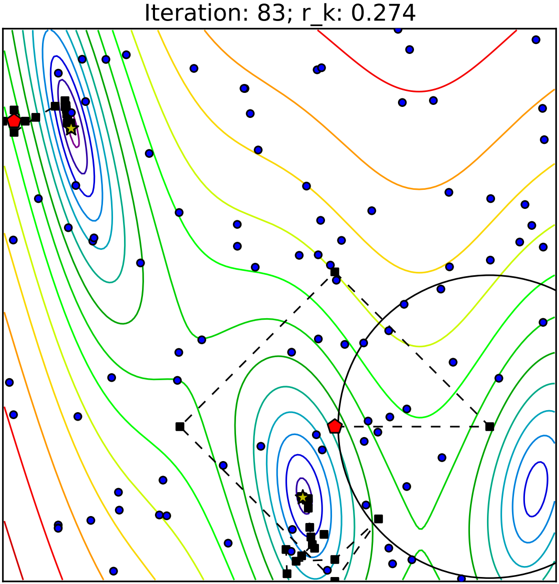

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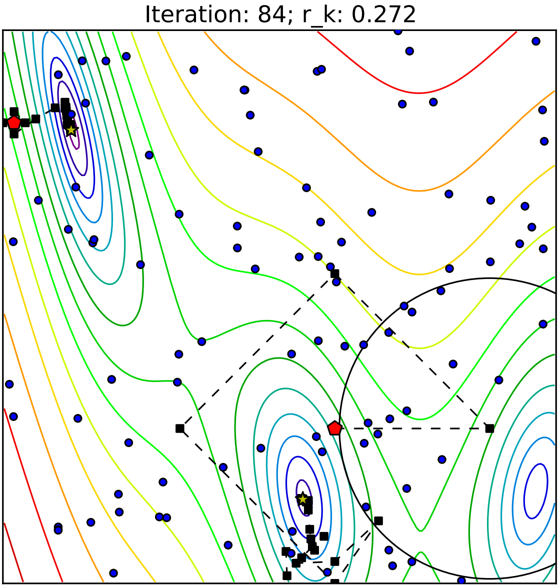

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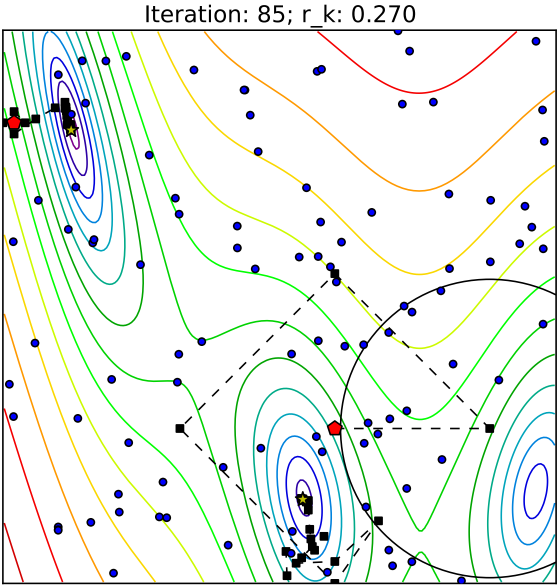

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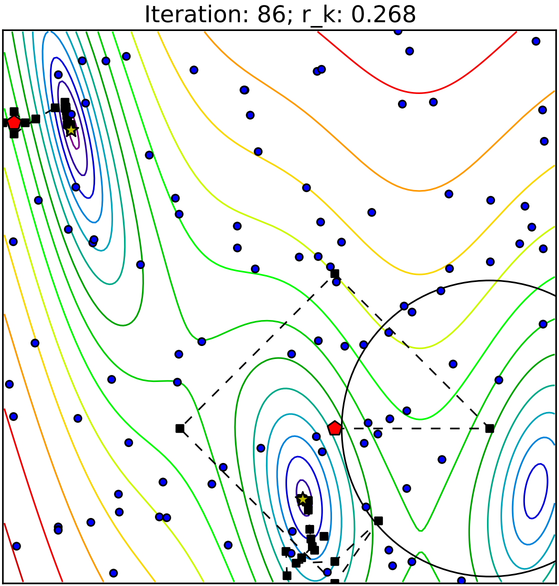

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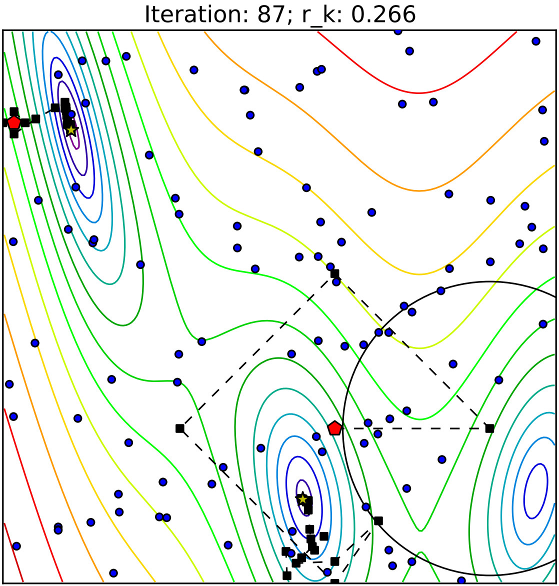

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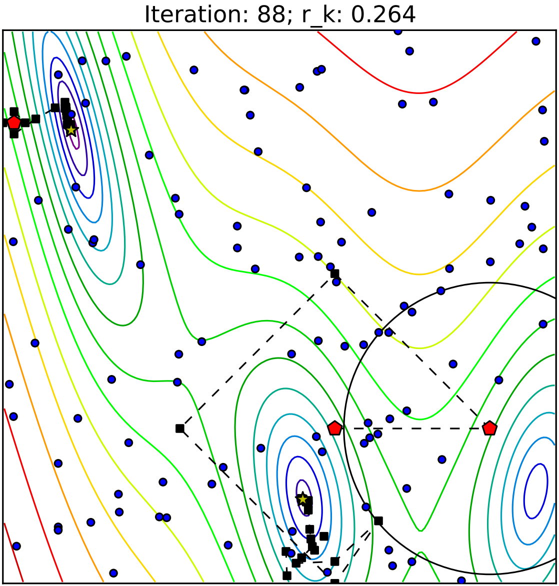

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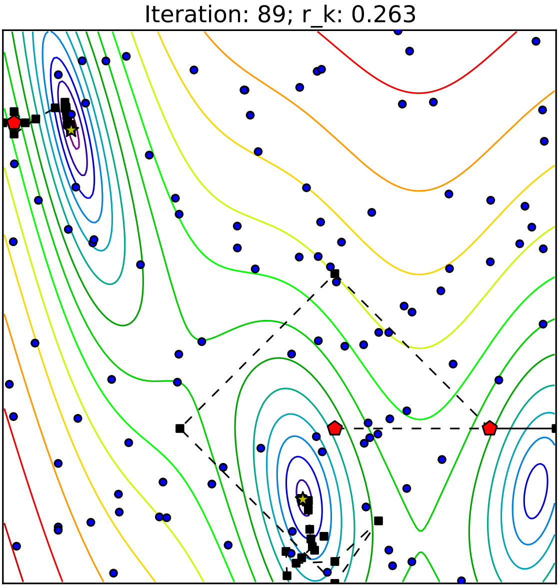

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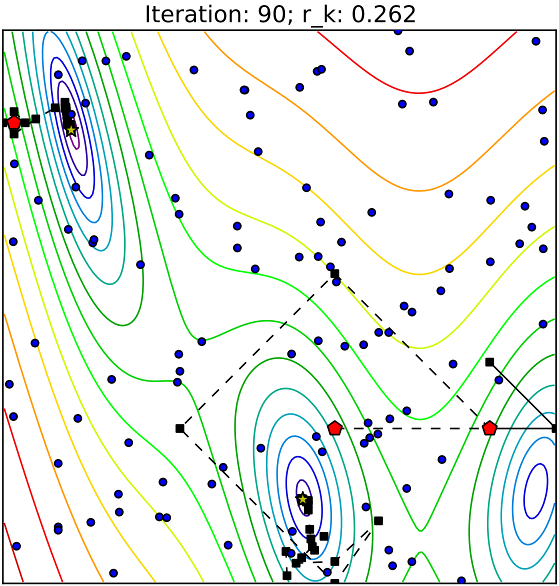

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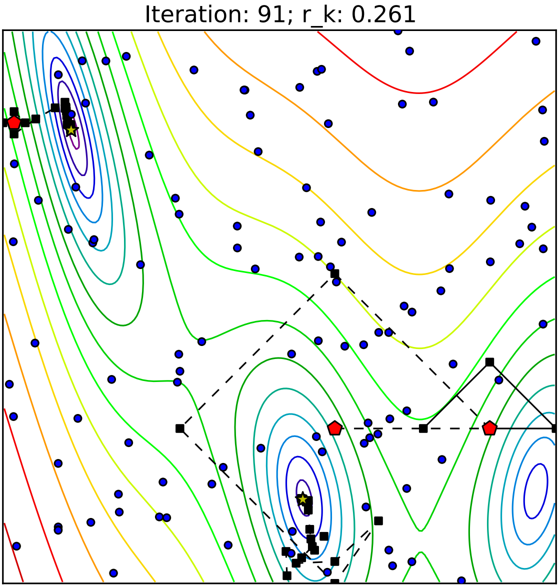

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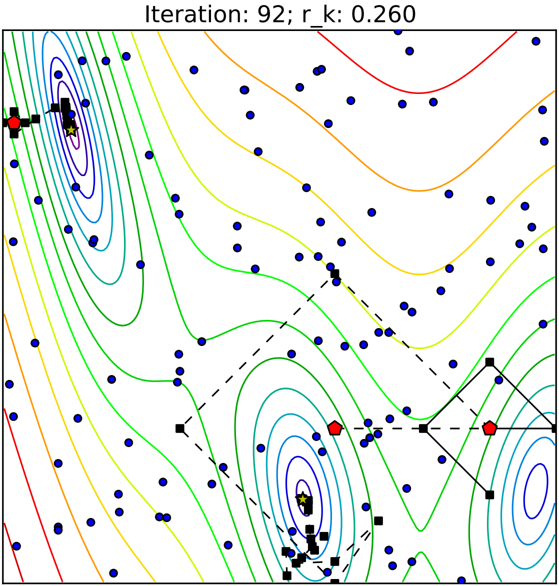

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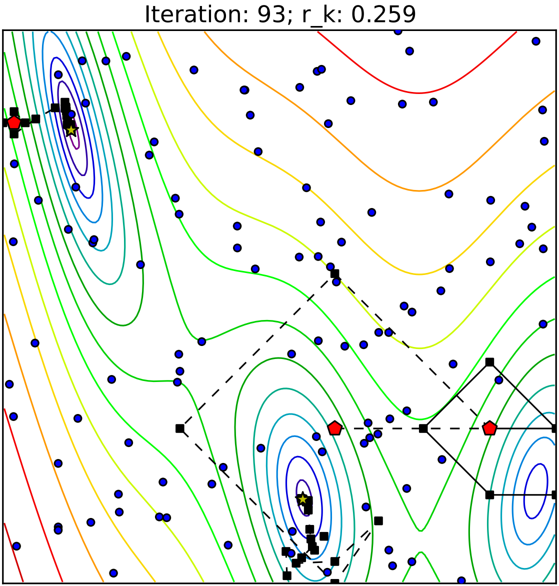

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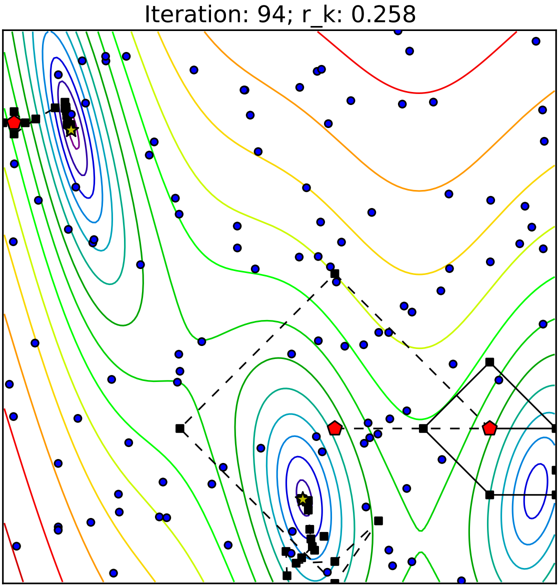

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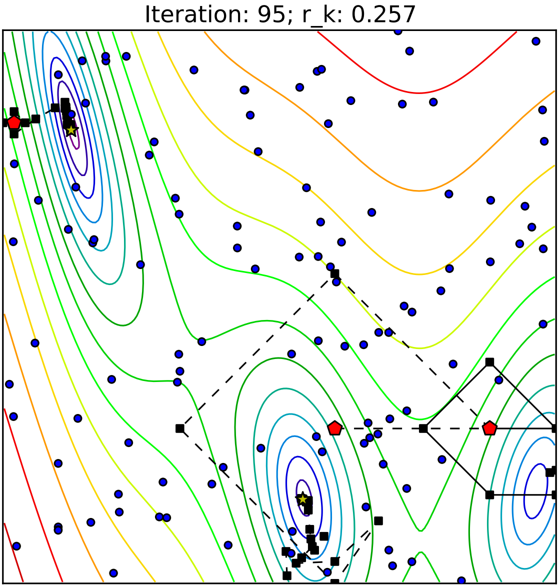

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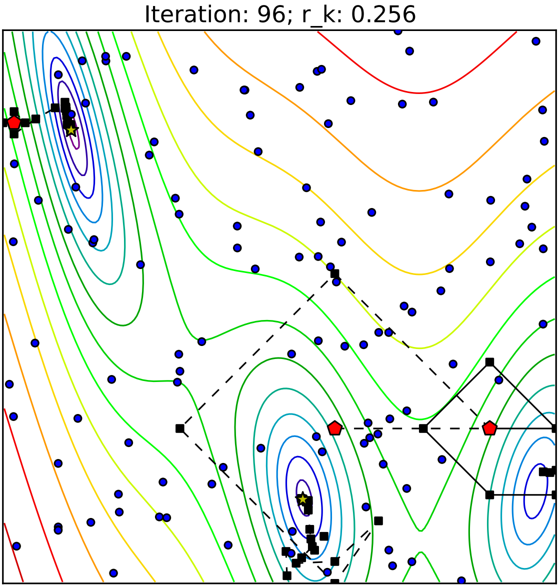

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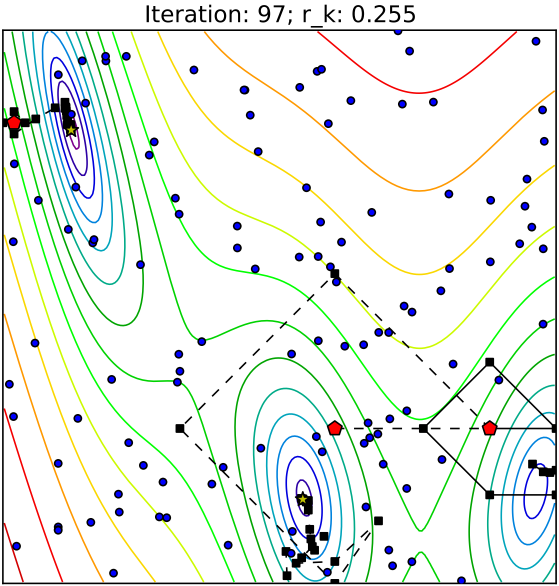

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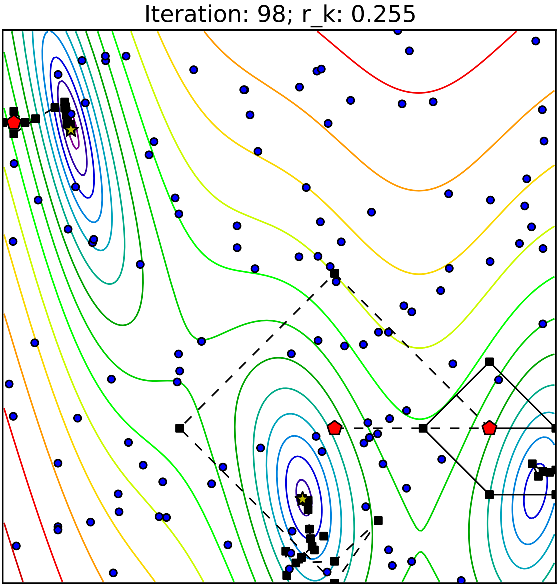

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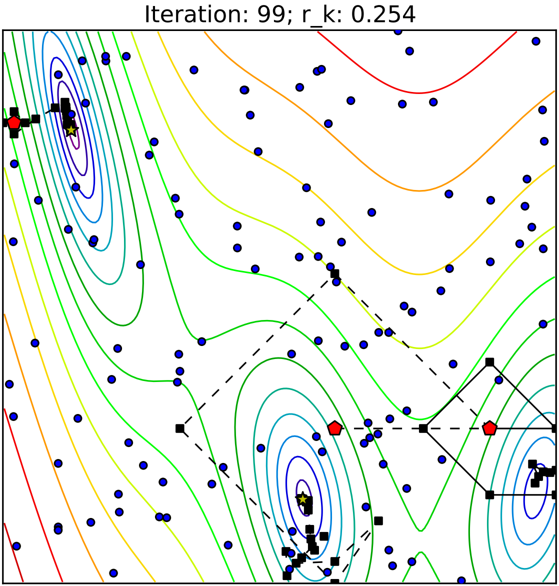

Properties of the local optimization method

Necessary:

- Honors a starting point
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ORBIT satisfies these [Wild, Regis, Shoemaker, SIAM-JOSC, 2008]

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Possibly beneficial:

- Can return multiple points of interest
- Reports solution quality/confidence at every iteration
- Can avoid certain regions in the domain
- Uses a history of past evaluations of f
- Uses additional points mid-run

APOSSM Theory

Theorem

Given the same assumptions as MLSL, APOSSM will start a finite number of local optimization runs with probability 1.

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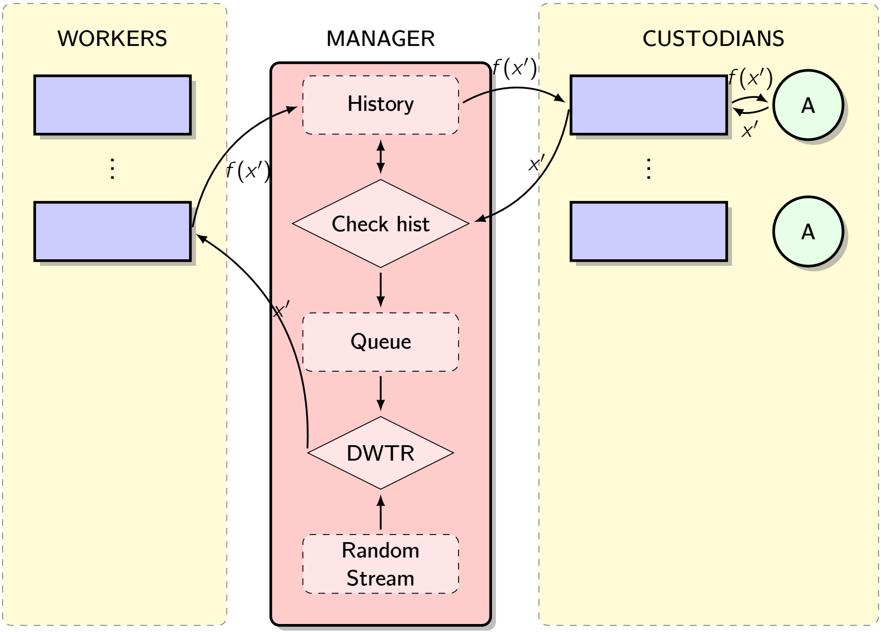
Theorem

Each $x^* \in X^*$ will almost surely be either identified in a finite number of evaluations or have a single local optimization run that is converging asymptotically to it.

Measuring Performance

- **GLODS** Global & local optimization using direct search [Custódio, Madeira (JOGO, 2014)]
- **Direct** Serial DIRECT [D. Finkel's MATLAB code]
- **pVTDirect** Parallel DIRECT [He, Watson, Sosonkina (TOMS, 2009)]
- **Random** Uniform sampling over domain (as a baseline)
- **POSMM**
  - Local optimization method
    - ORBIT [Wild, Regis, & Shoemaker (SIAM JOSC, 2008)]
    - BOBYQA [Powell, 2009]
  - Initial sample size: $10n$

- Each method evaluates Direct's $2n + 1$ initial points.



(A)POSMM Diagram

(A)POSMM Manager

Algorithm 3: Manager Logic

while $k < \text{fevalmax}$ **do**
    MPI.recv(MPI.ANY_SOURCE)
    if *Received from Custodian* **then**
        Check H_k
        Add new point to Q_L
    if *Received from Worker* **then**
        Update H_k
        Possibly get a Custodian working on the next point
        Run `decide_where_to_start`
        Possibly update Q_L
    if sync=False *OR All Workers/Custodians are done* **then**
        Give from Q_L or $\mathcal{R}_S$ to available worker(s)

POSMM

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(L4) $\hat{x}$ is at least μ from $\partial\mathcal{D}$ and ν from known local minima

(L5) $\hat{x}$ is not in an active local optimization run and has not been ruled stationary

(L6) $\exists r_k$-descent path in H_k from some $x \in S_k$ satisfying (S2-S4) to $\hat{x}$

Measuring Performance

Notation:

Let X^* be the set of all local minima of f.
Let $f^*_{(i)}$ be the ith smallest value $\{f(x^*)|x^* \in X^*\}$.
Let $x^*_{(i)}$ be the element of X^* corresponding to the value $f^*_{(i)}$.

The global minimum has been found at a level $\tau > 0$ at batch k if an algorithm it has found a point $\hat{x}$ satisfying:

$$f(\hat{x}) - f^*_{(1)} \leq (1 - \tau)\left(f(x_0) - f^*_{(1)}\right),$$

where x_0 is the starting point for problem p.

Measuring Performance

Notation:

Let X^* be the set of all local minima of f.
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The j best local minima have been found at a level $\tau > 0$ at batch k if:

$$\left|\left\{x^*_{(1)}, \ldots, x^*_{(\underline{j}-1)}\right\} \bigcap \left\{x^*_{(i)} : \exists x \in H_k \text{ with } \left\|x - x^*_{(i)}\right\| \le r_n(\tau)\right\}\right| = \underline{j} - 1$$

$$\&$$

$$\left|\left\{x^*_{(\underline{j})}, \ldots, x^*_{(\bar{j})}\right\} \bigcap \left\{x^*_{(i)} : \exists x \in H_k \text{ with } \left\|x - x^*_{(i)}\right\| \le r_n(\tau)\right\}\right| \ge j - \underline{j} + 1,$$

where $\underline{j}$ and $\bar{j}$ are the smallest and largest integers such that $f^*_{(\bar{j})} = f^*_{(j)} = f^*_{(\underline{j})}$ and where $r_n(\tau) = \sqrt[n]{\frac{\tau \operatorname{vol}(\mathcal{D})\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$.

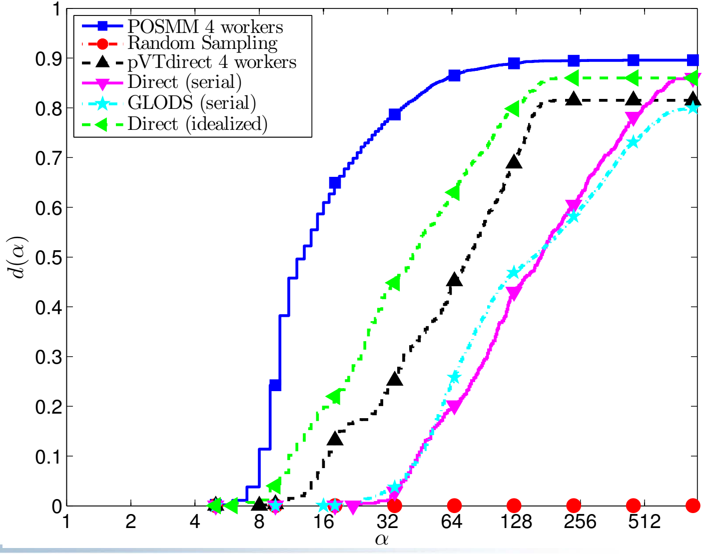
Problems considered

GKLS problem generator [Gaviano et al., "Algorithm 829" (TOMS, 2003)]

- 600 synthetic problems with known local minima
- $n = 2, \dots, 7$
- 10 local minima in the unit cube with a unique global minimum
- 100 problems for each dimension
- 5 replications (different seeds) for each problem
- 5000 evaluations

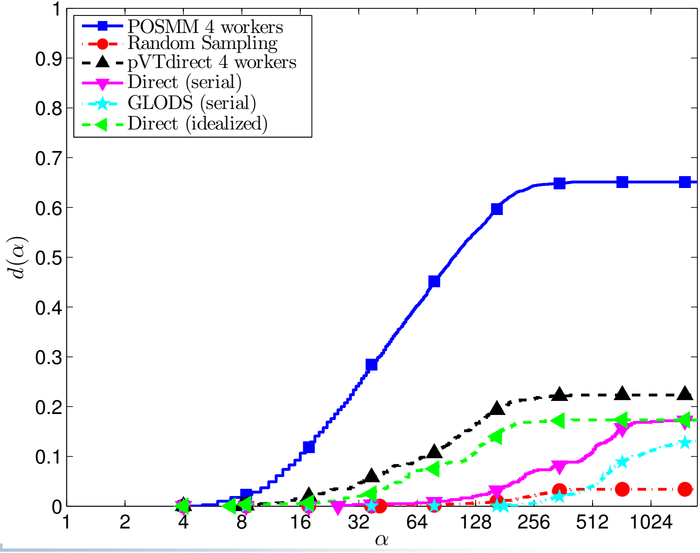
Data Profiles

$$f(x) - f^*_{(1)} \le (1 - 10^{-5}) \left(f(x_0) - f^*_{(1)} \right)$$

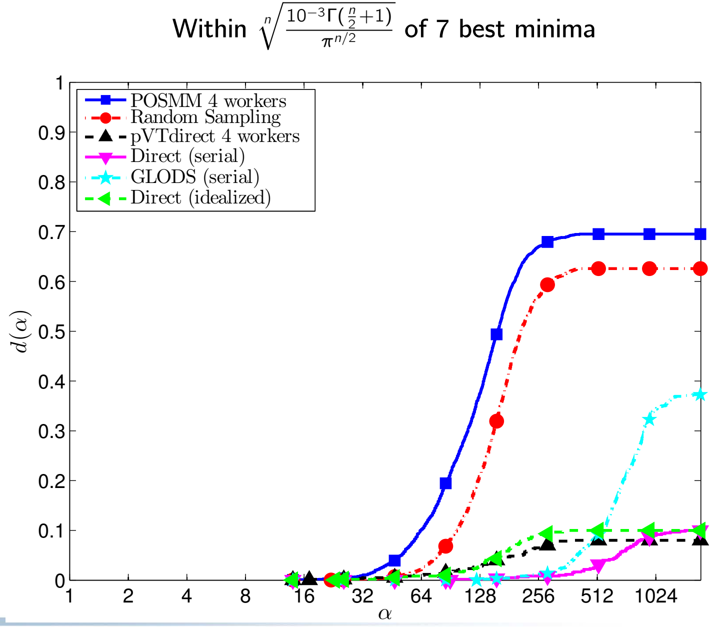


Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 3 best minima

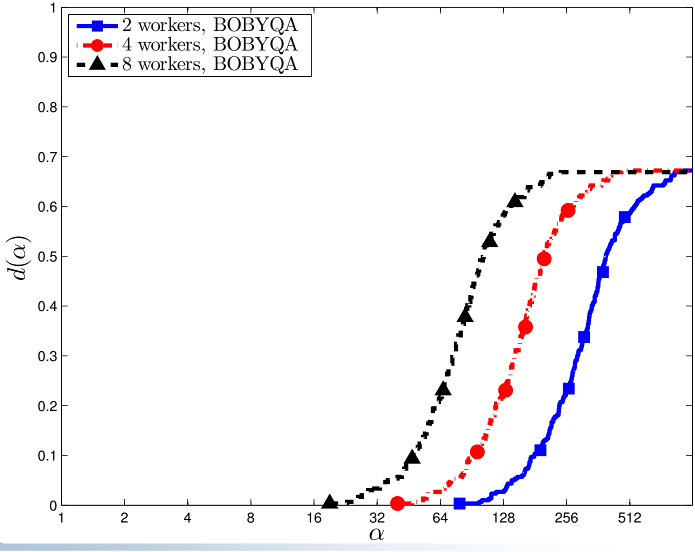


Data Profiles



Data Profiles (increasing workers)

Within $\sqrt[n]{\frac{10^{-3}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 7 best minima



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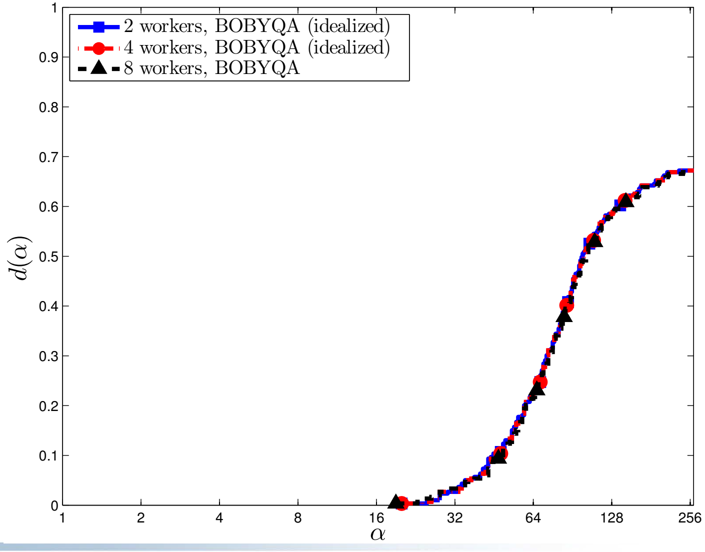

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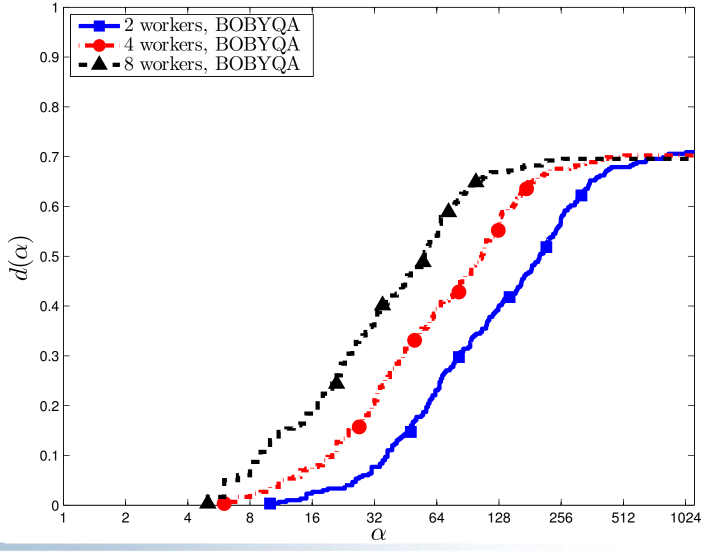

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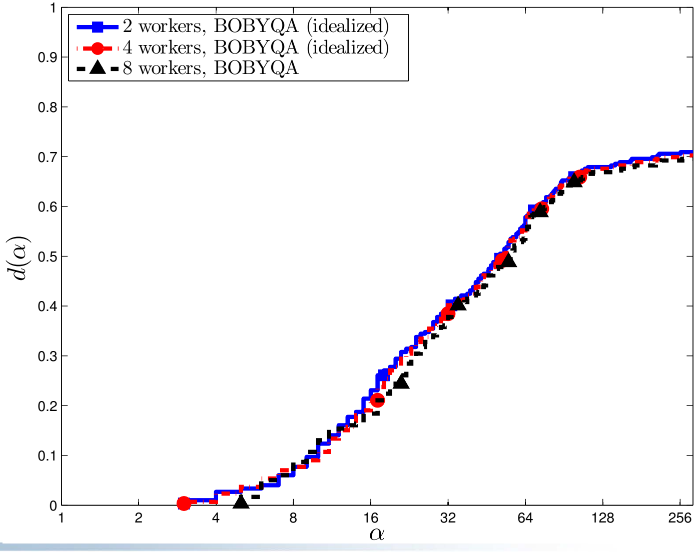

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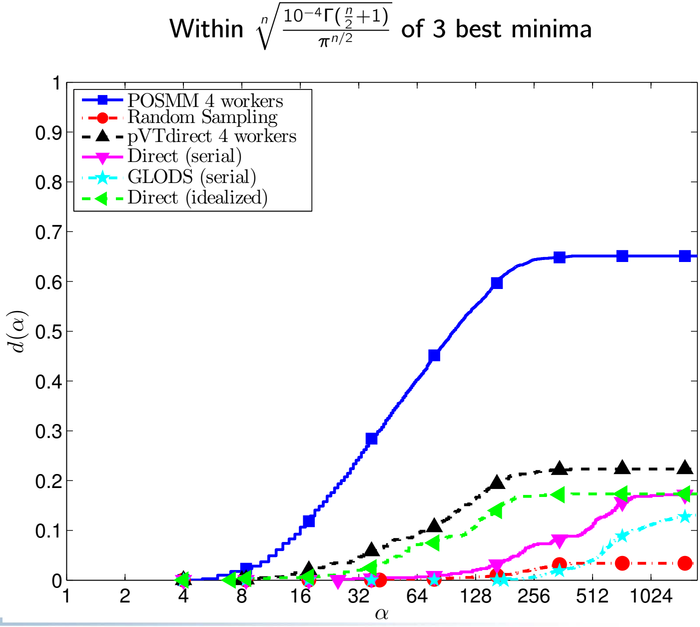

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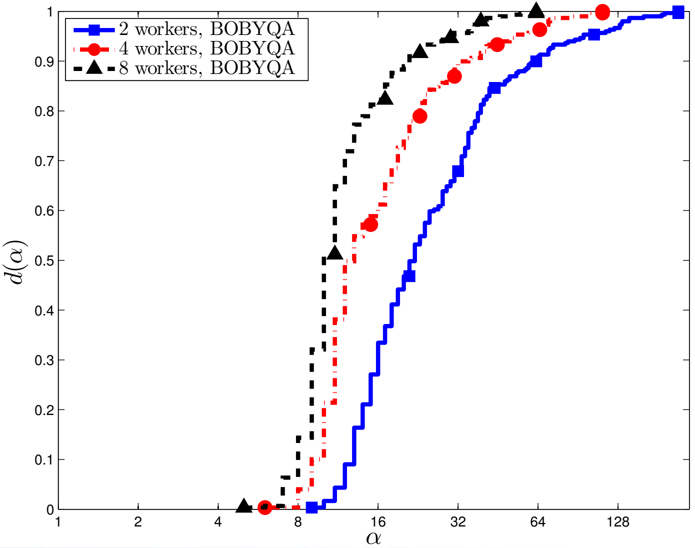

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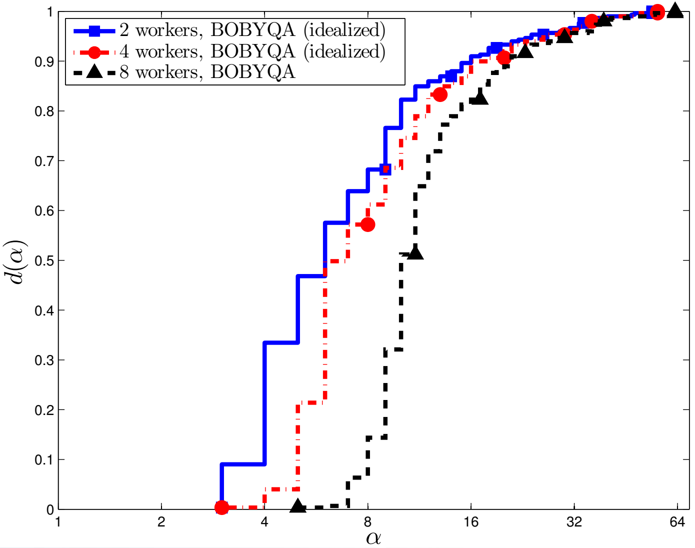
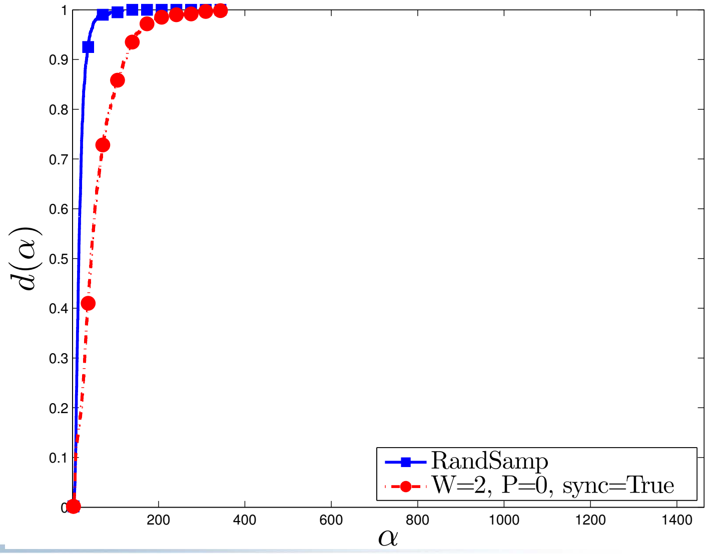
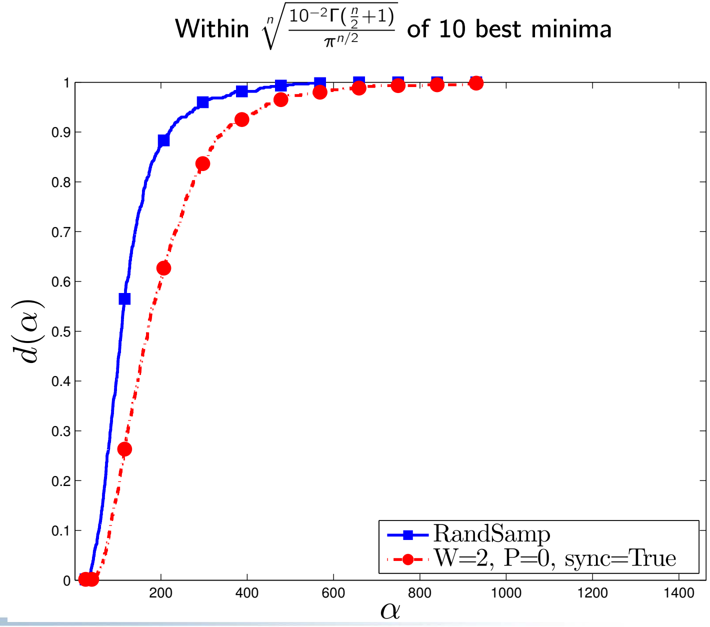


Data Profiles (vs random)

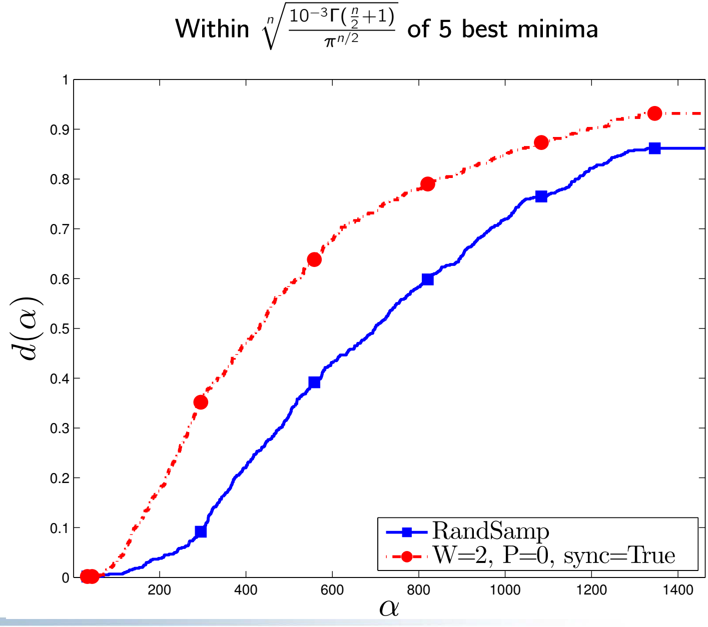
Within $\sqrt[n]{\frac{10^{-1}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 10 best minima



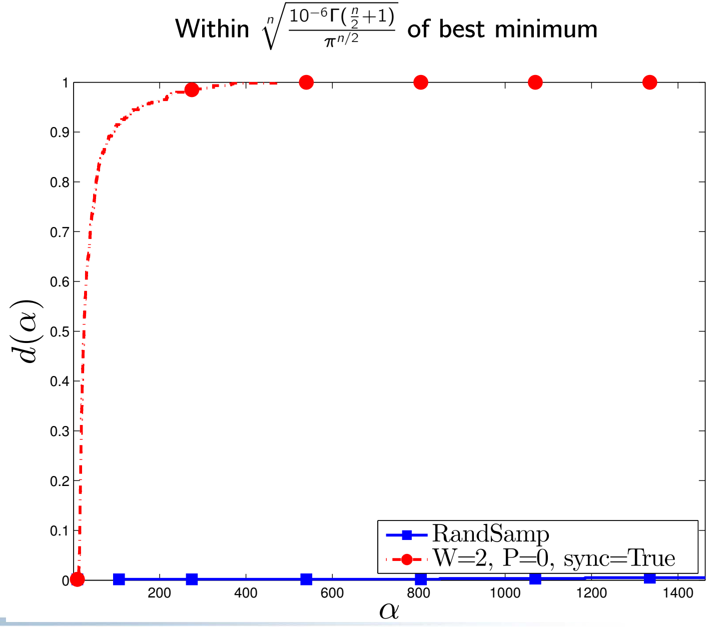
Data Profiles (vs random)



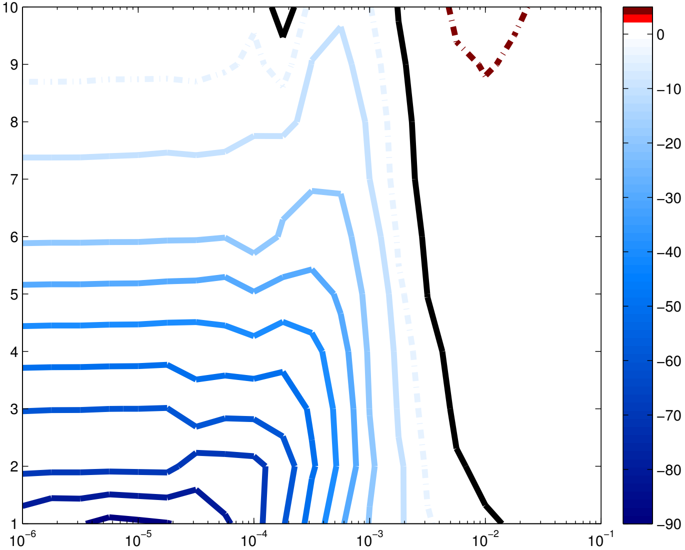
Data Profiles (vs random)



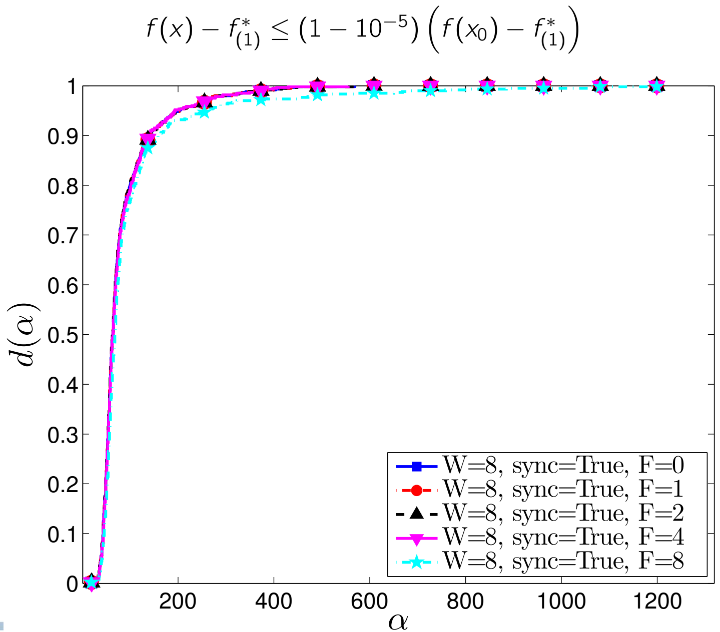
Data Profiles (vs random)



Data Profiles (vs random)

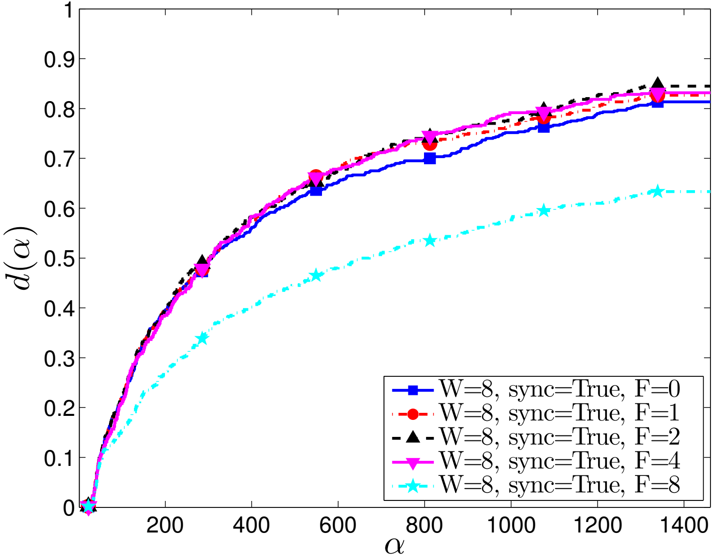


Data Profiles (forcing runs)



Data Profiles (forcing runs)

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 3 best minima



Closing Remarks

- Concurrent function evaluations can locate multiple minima while efficiently finding a global minimum.

Closing Remarks

- Concurrent function evaluations can locate multiple minima while efficiently finding a global minimum.

- The ability to find many minima scales well with the number of workers.

Questions:

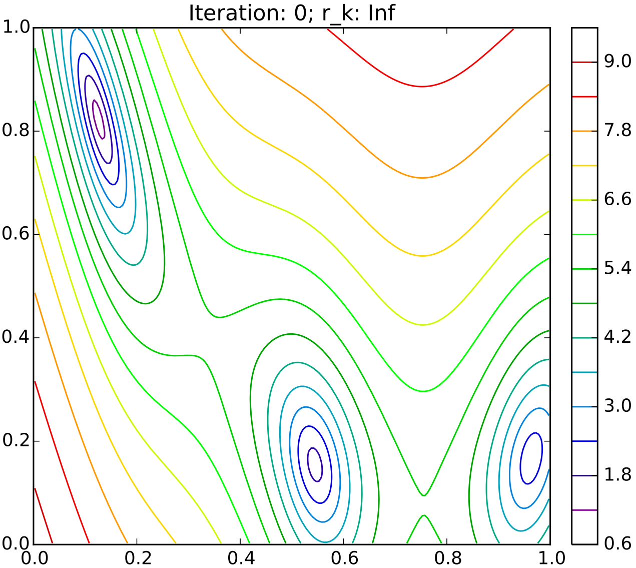
- Finding (or designing) the best local solver for our framework?
- Best way to process the queue?

(A)POSMM Manager

Algorithm 3: Manager Logic

while $k <$ fevalmax **do**
- MPI.recv(MPI.ANY_SOURCE)
- **if** *Received from Custodian* **then**
  - Check H_k
  - Add new point to Q_L
- **if** *Received from Worker* **then**
  - Update H_k
  - Possibly get a Custodian working on the next point
  - Run `decide_where_to_start`
  - Possibly update Q_L
- **if** sync=False *OR All Workers/Custodians are done* **then**
  - Give from Q_L or $\mathcal{R}_S$ to available worker(s)

Pausing runs



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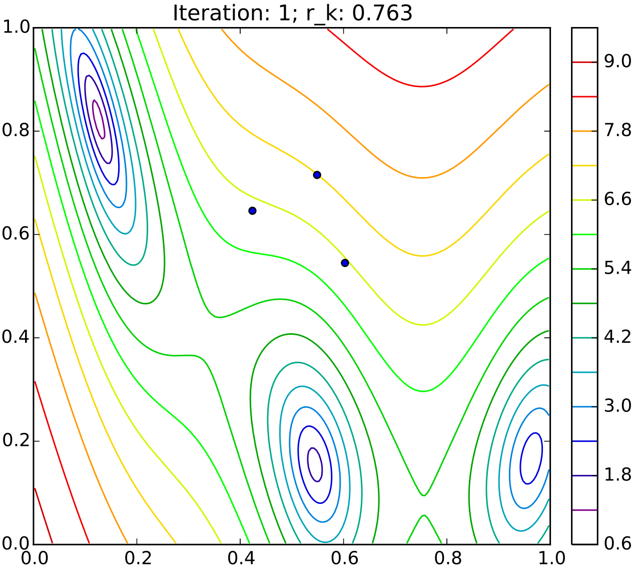

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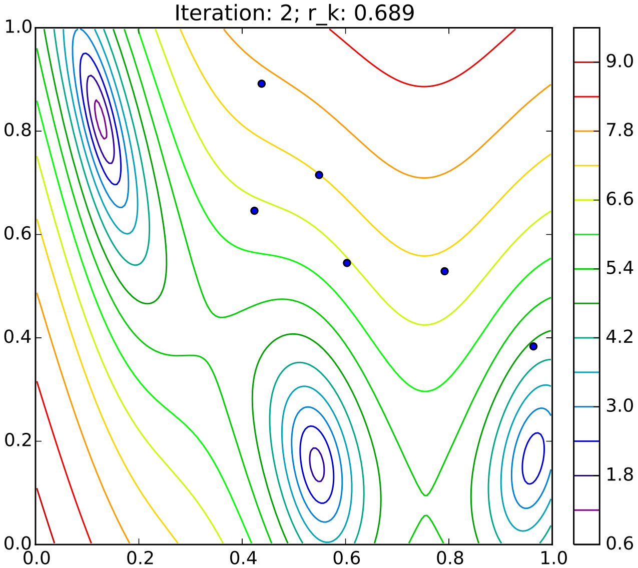
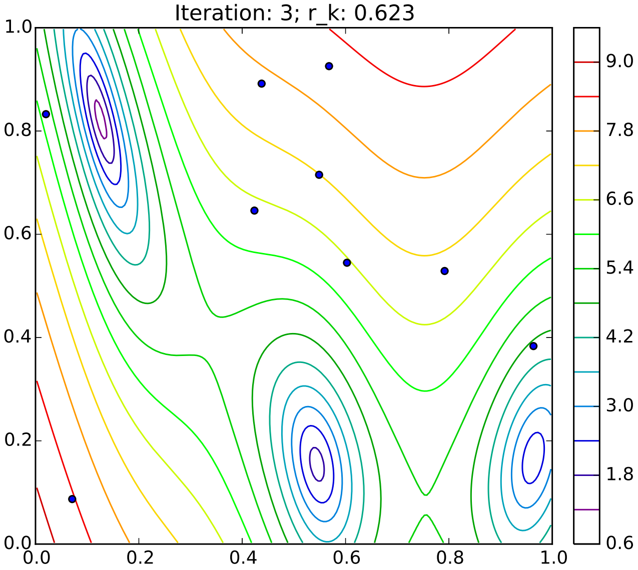


Pausing runs



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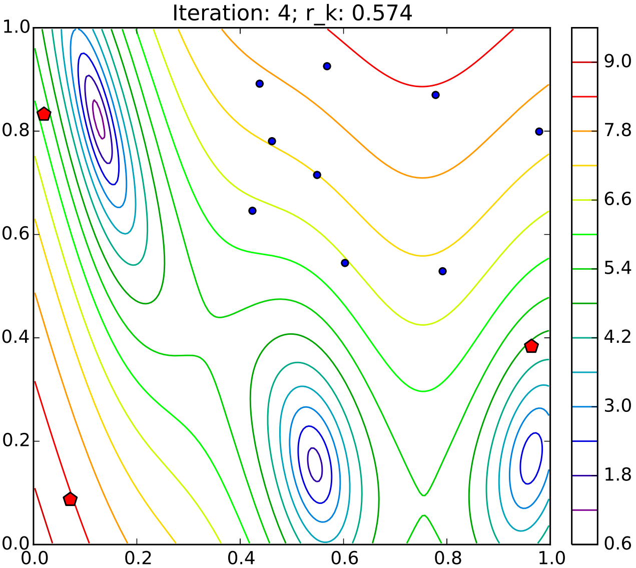

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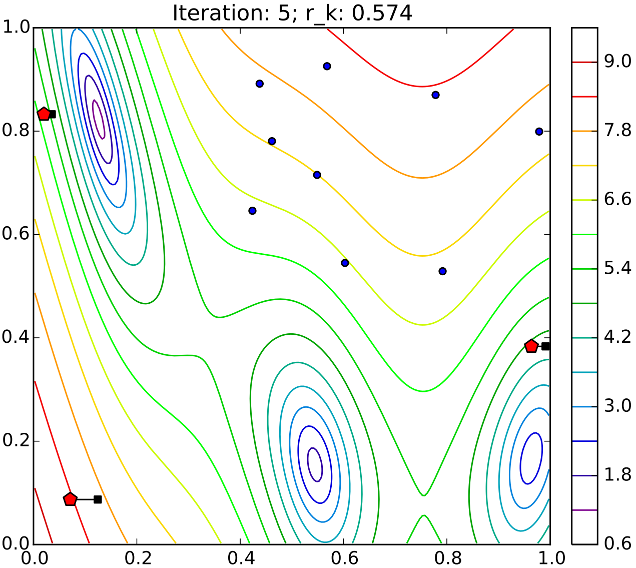

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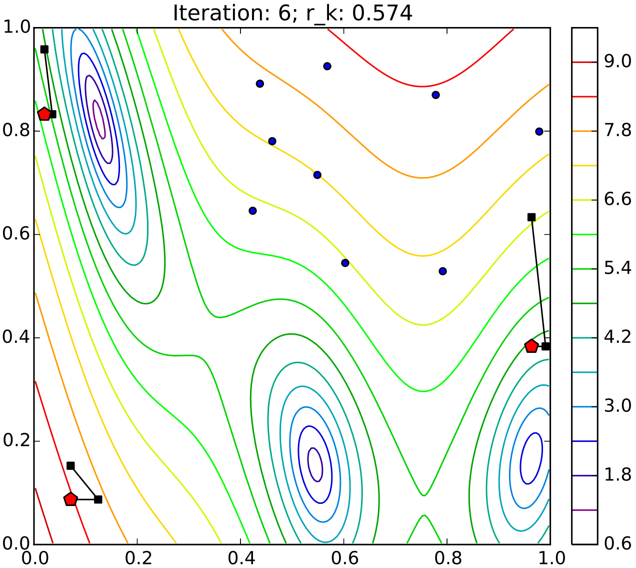

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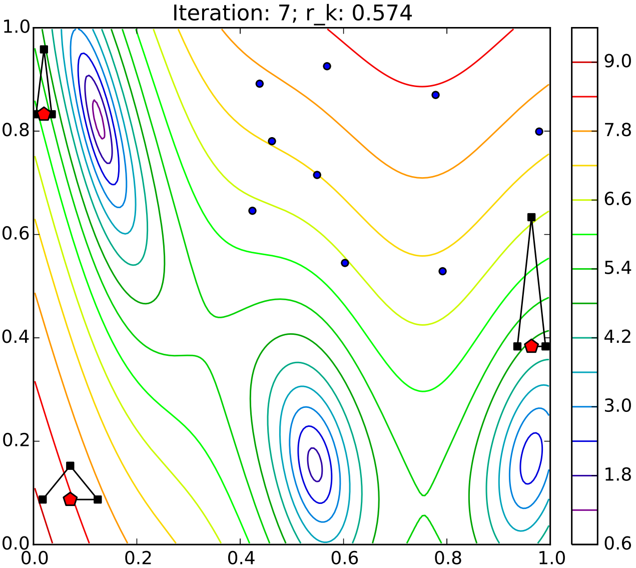

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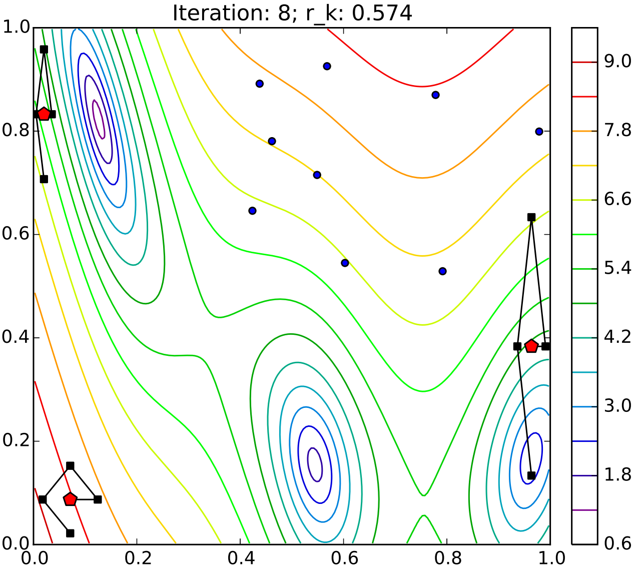

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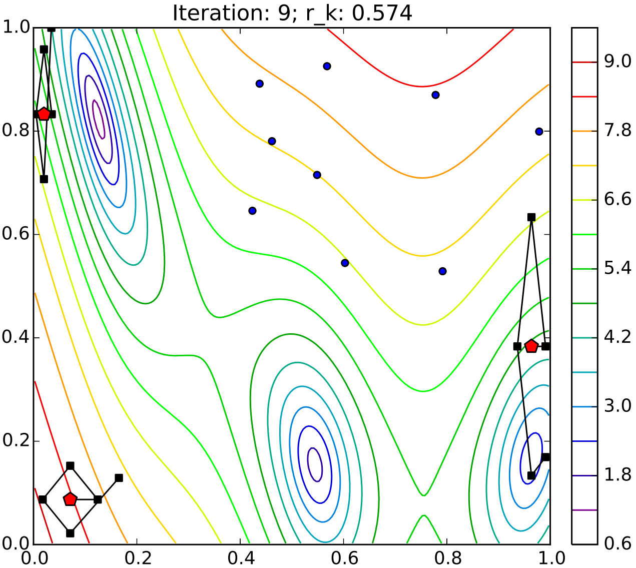

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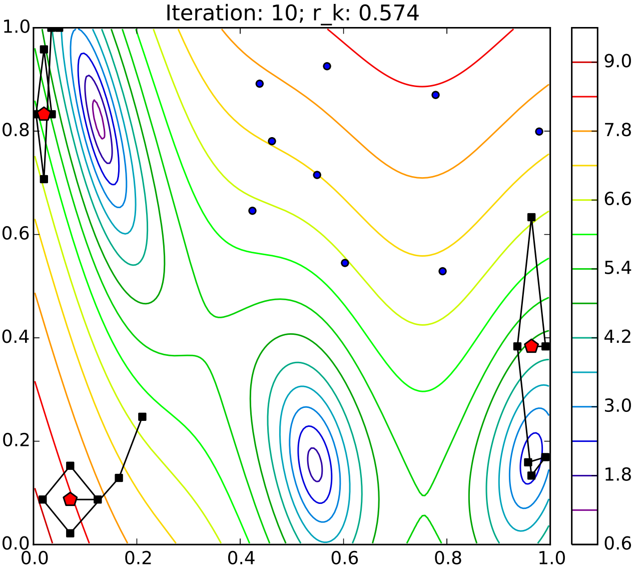

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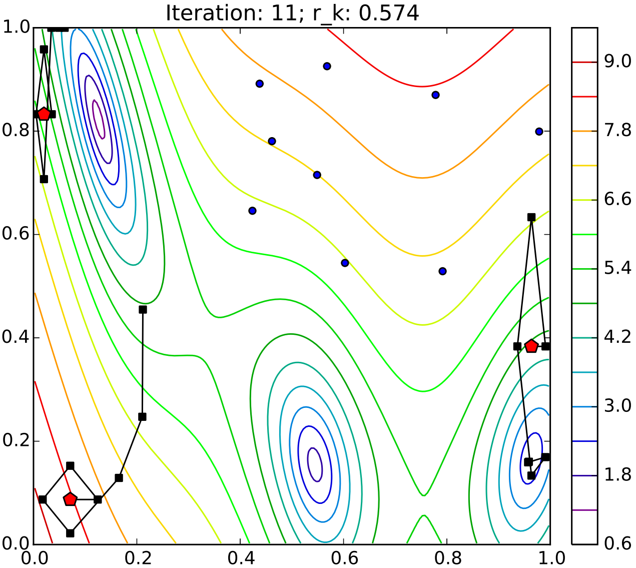

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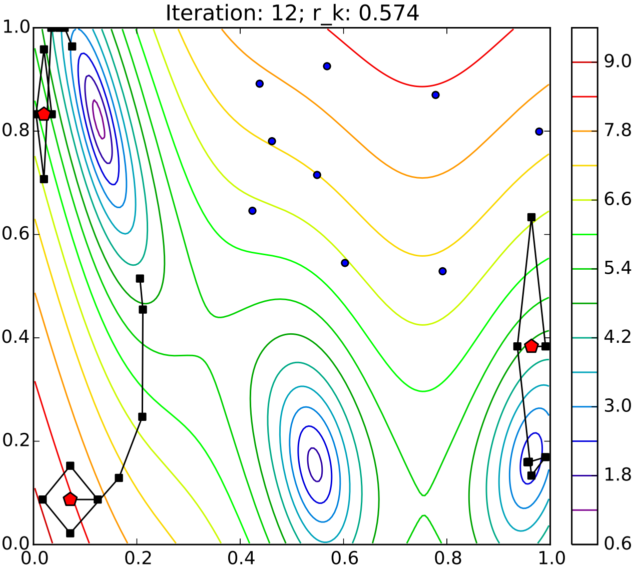

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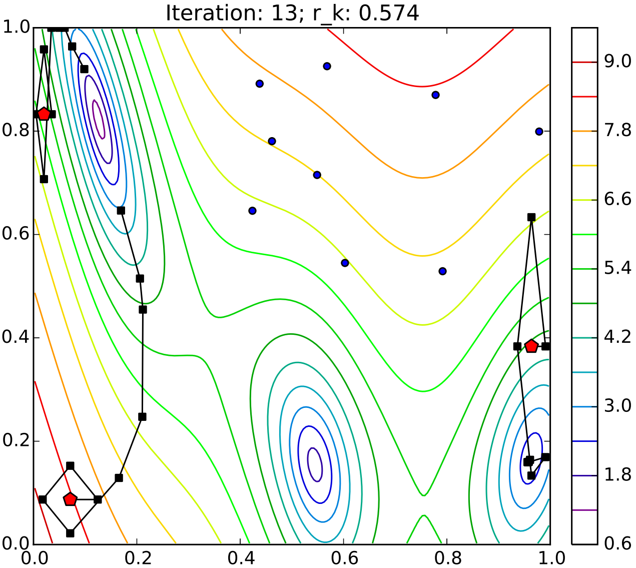

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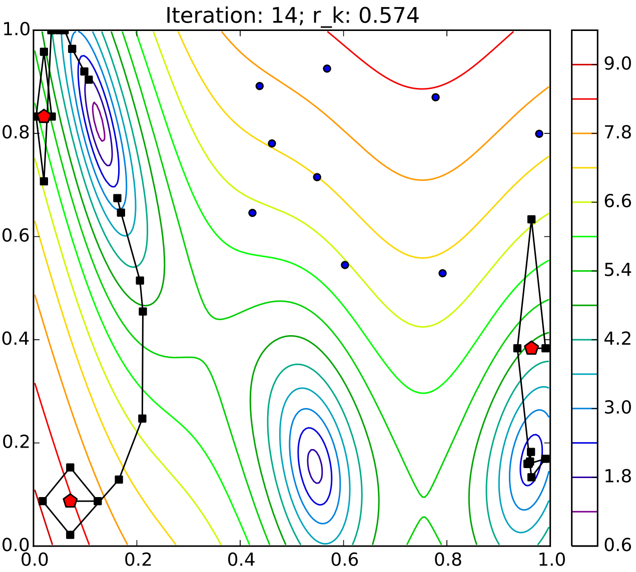

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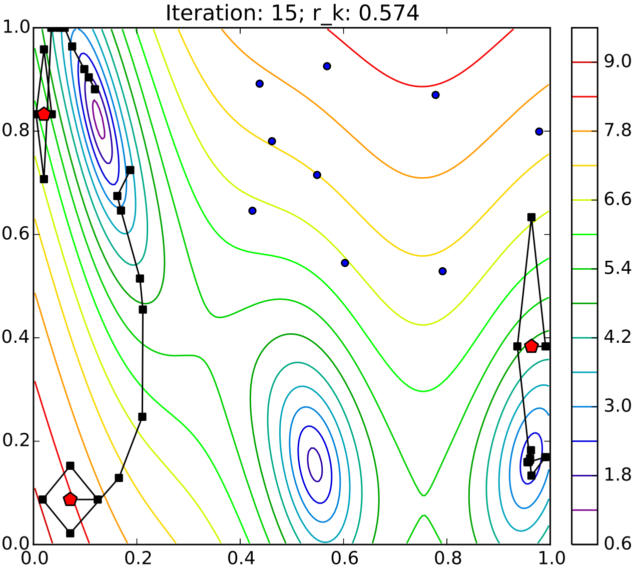

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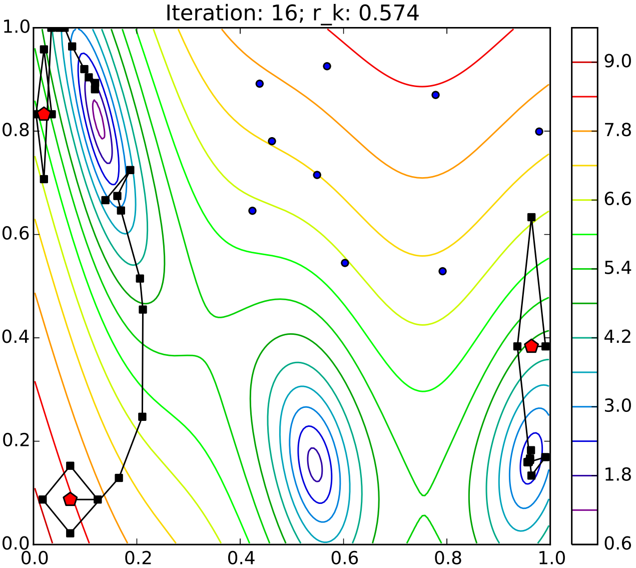

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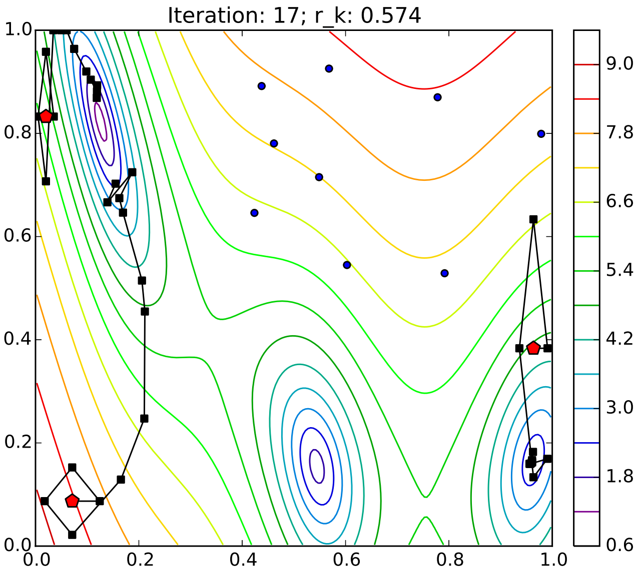

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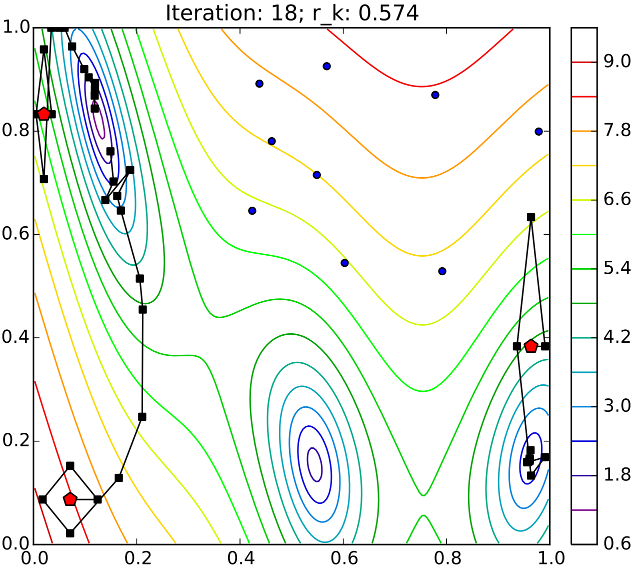

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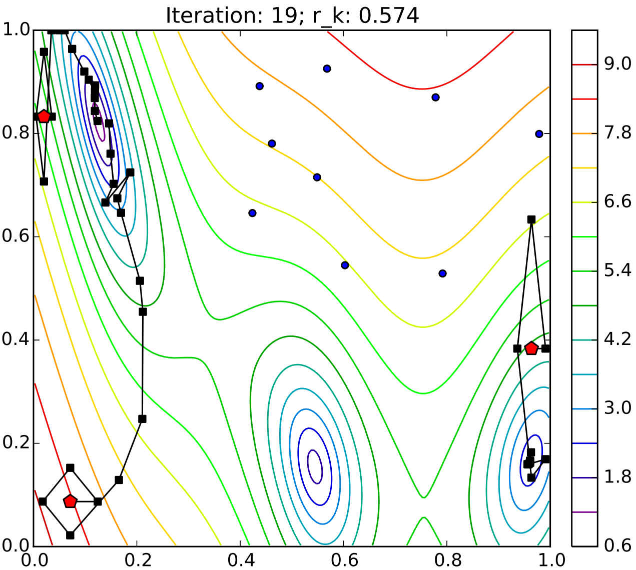

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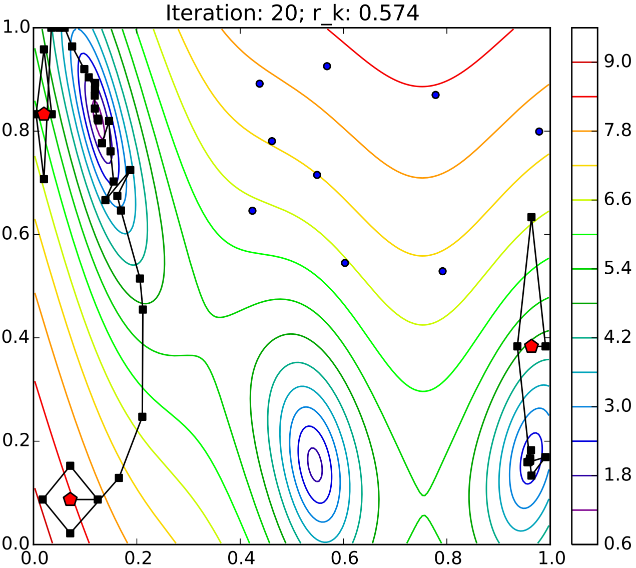

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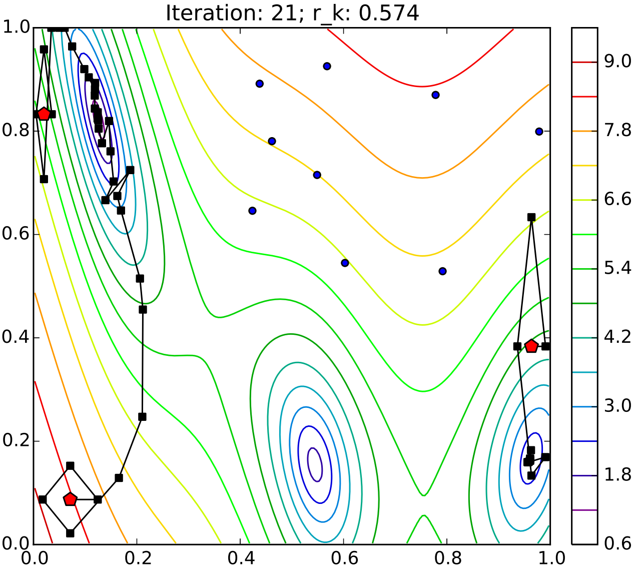

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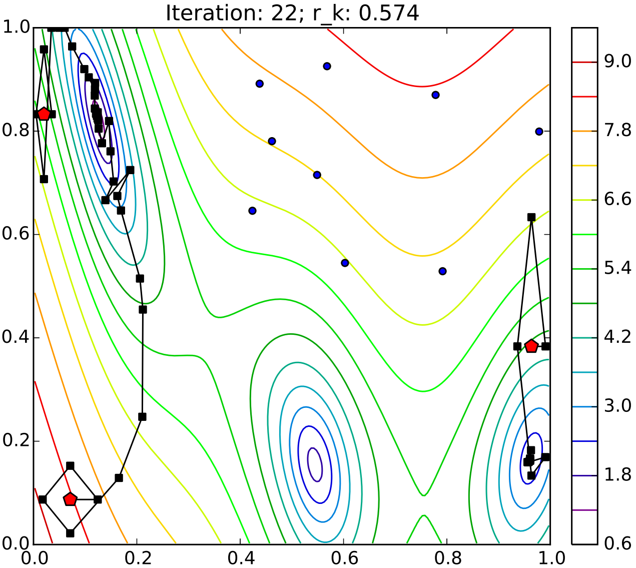

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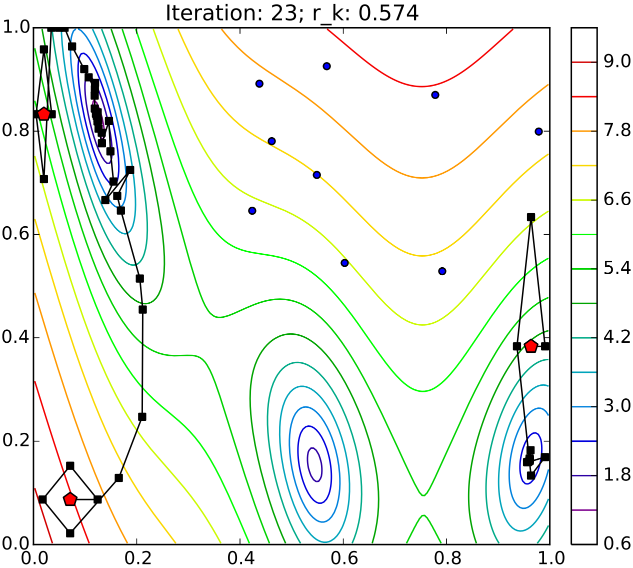

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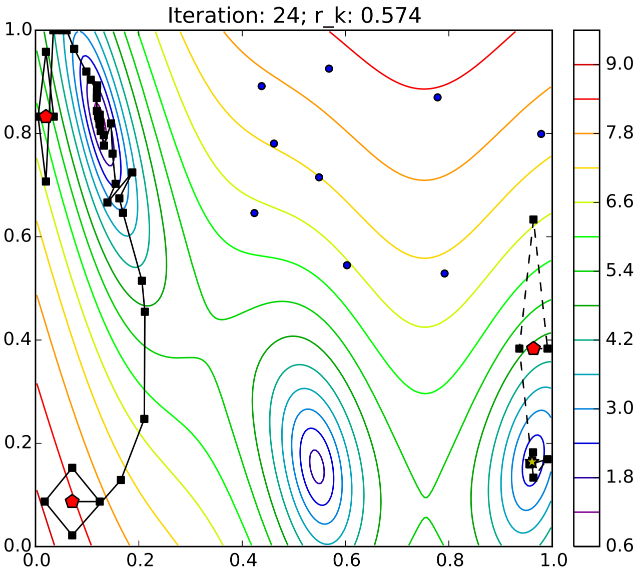

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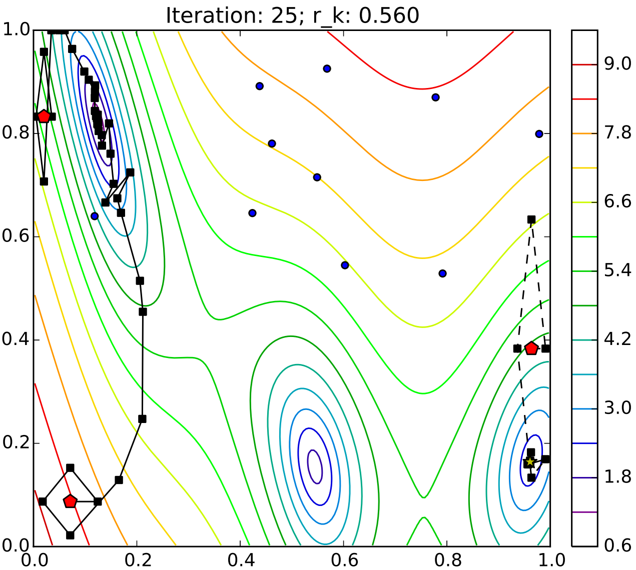

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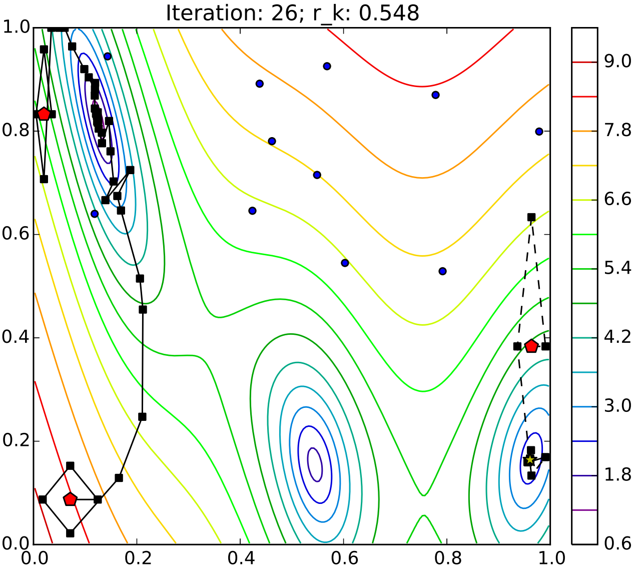

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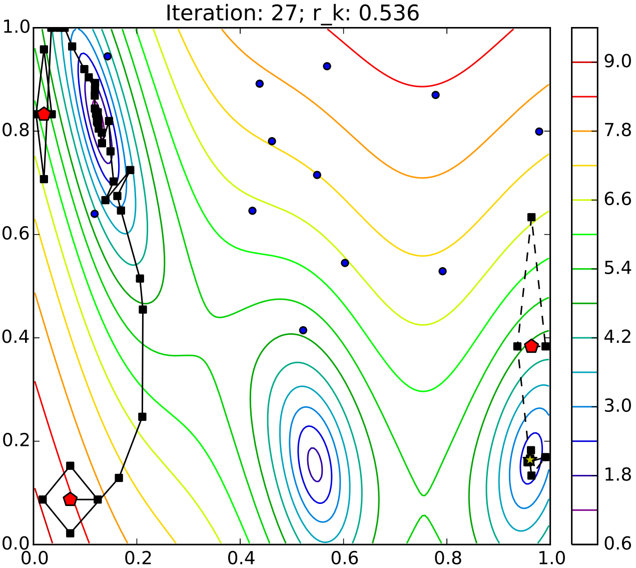

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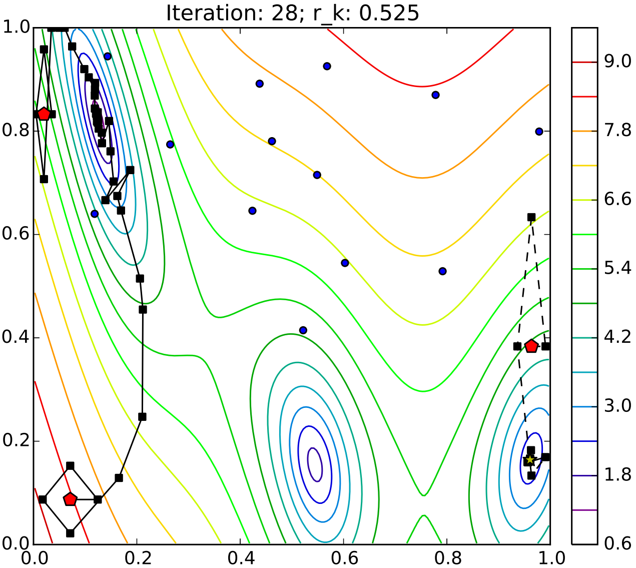

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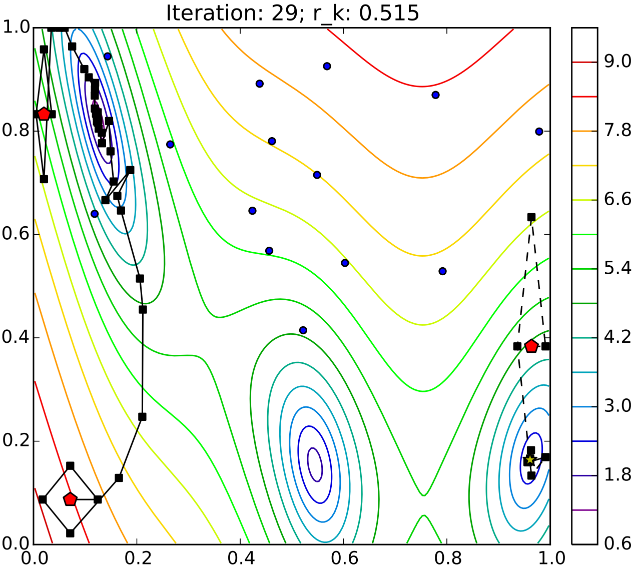

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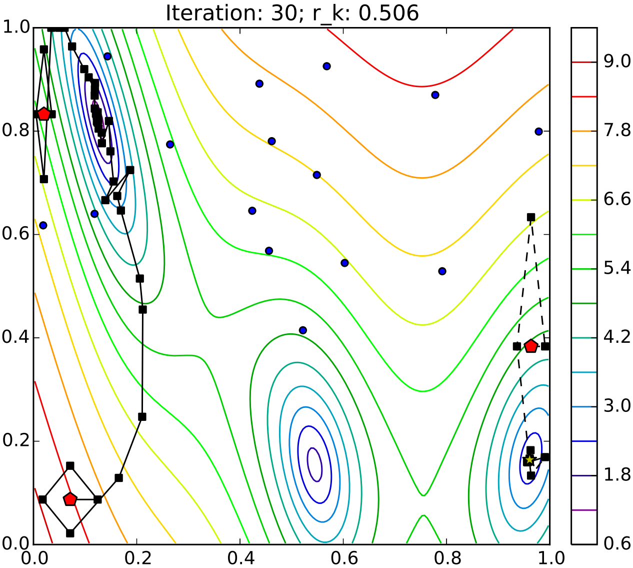

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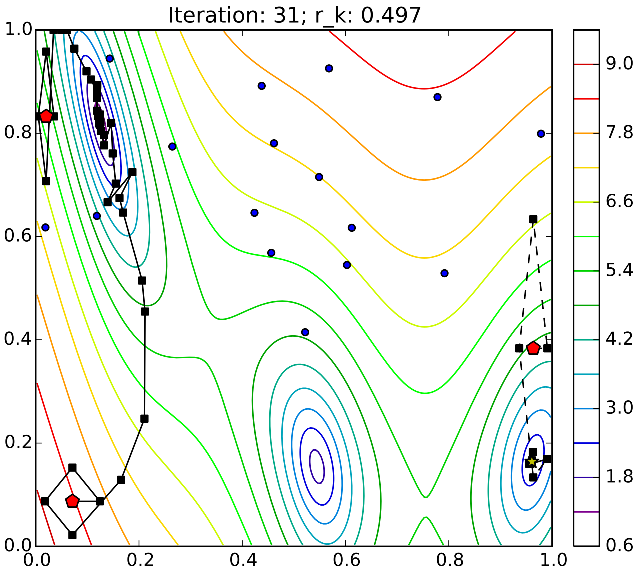

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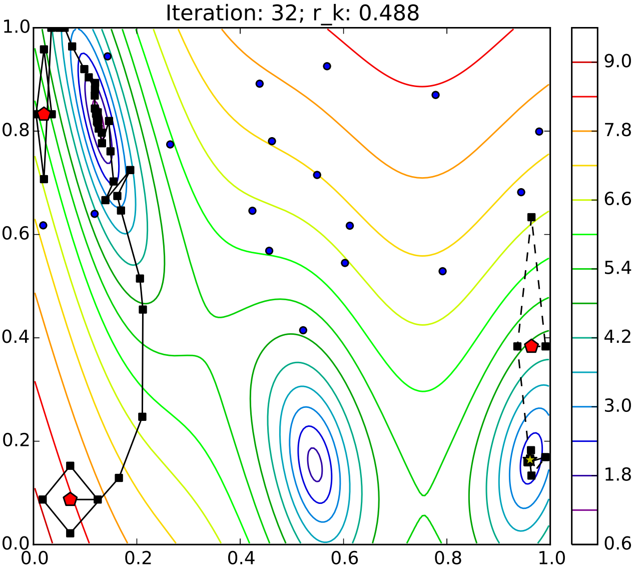

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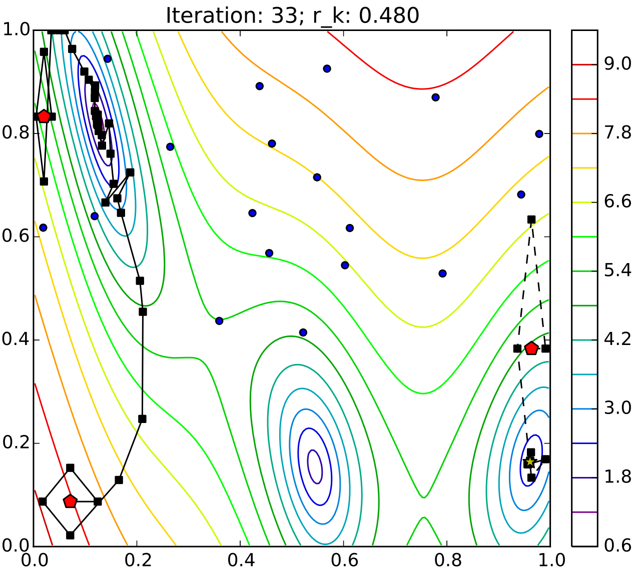

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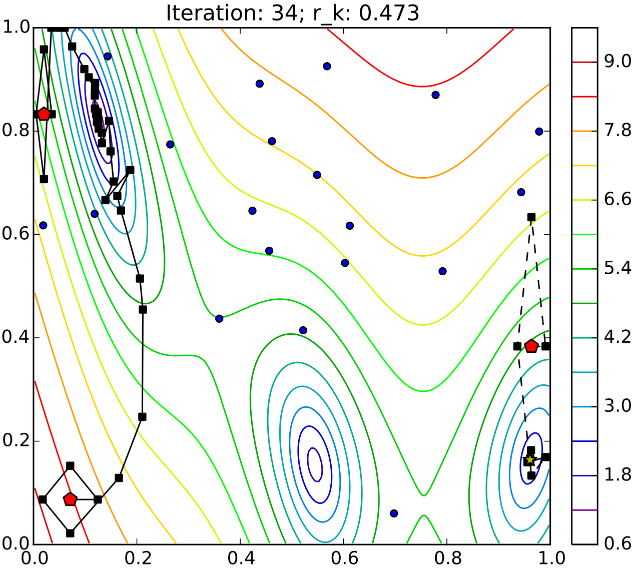

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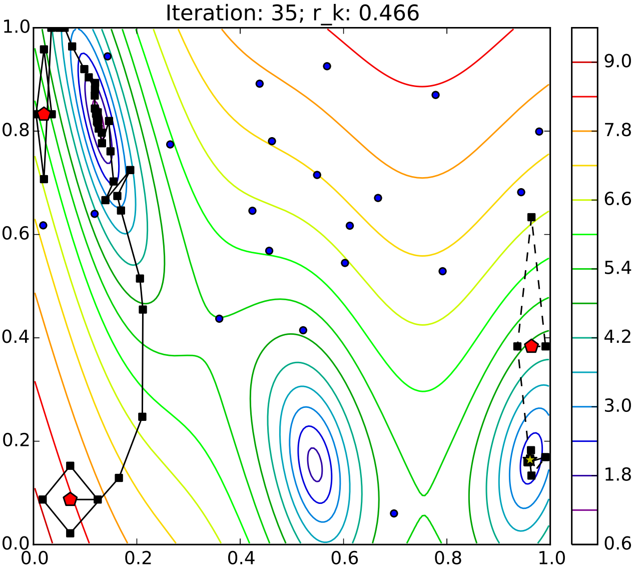

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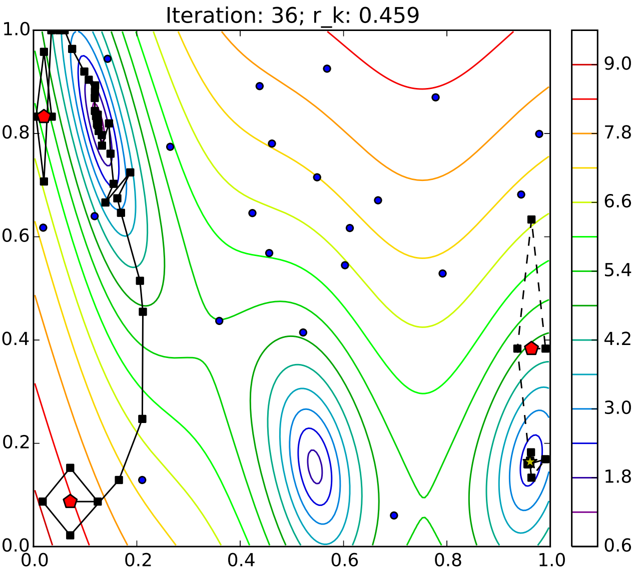

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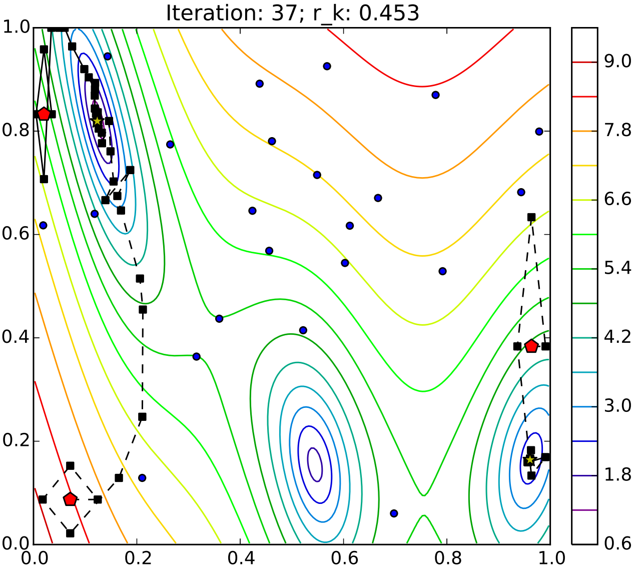

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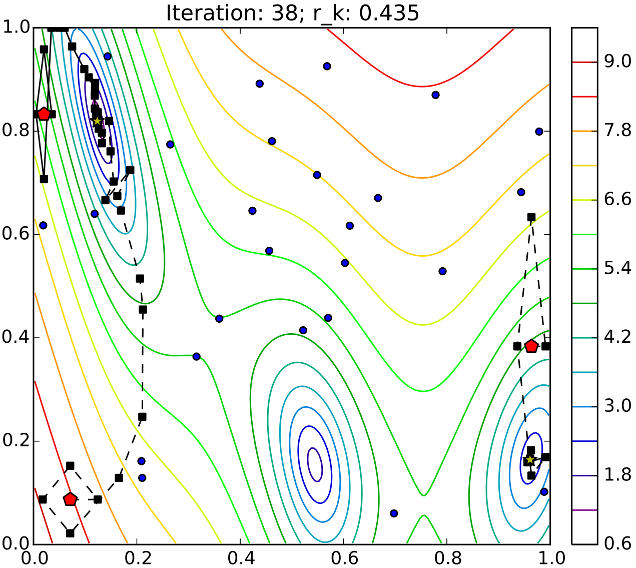

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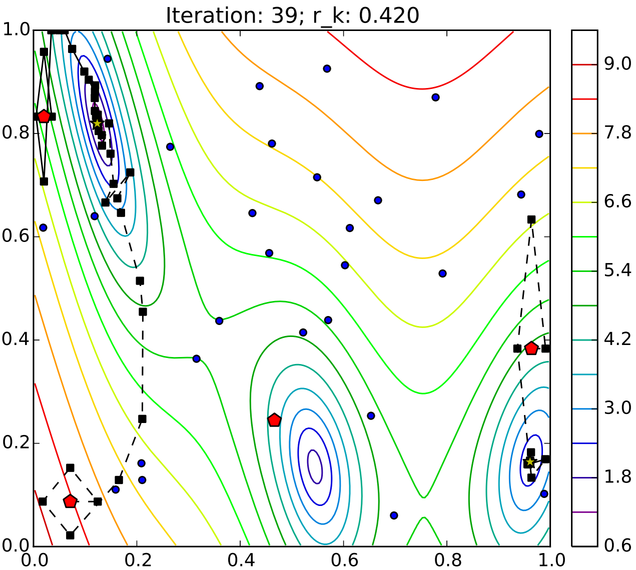
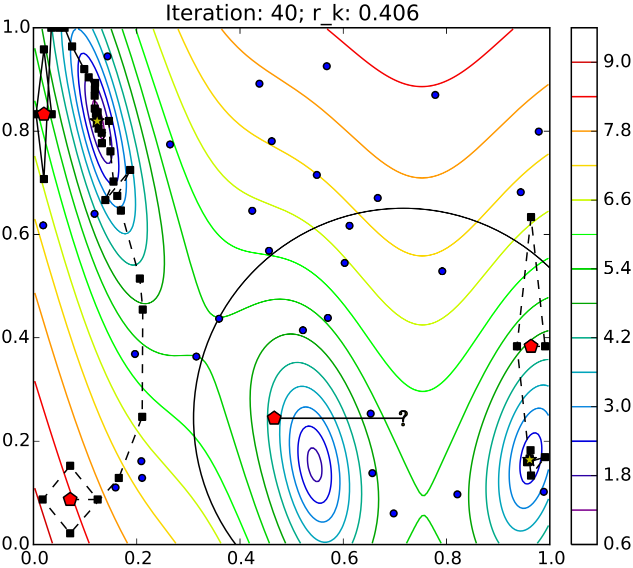
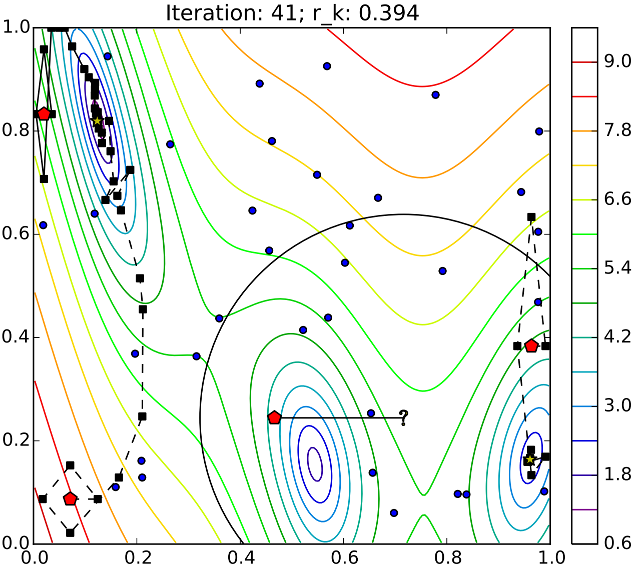


Pausing runs



Pausing runs



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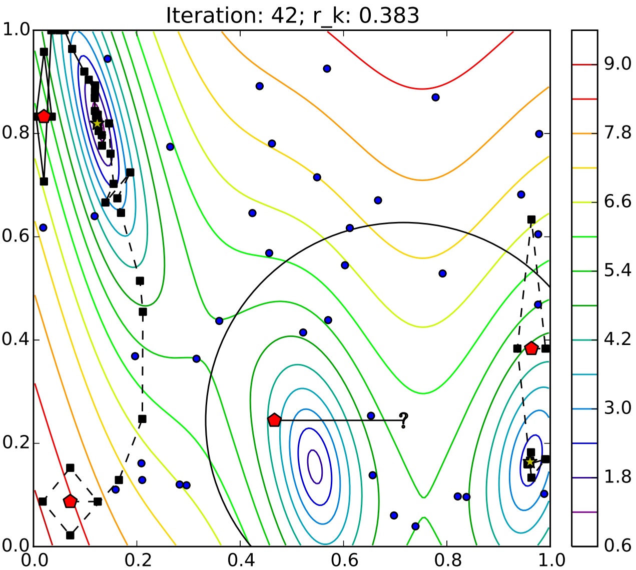
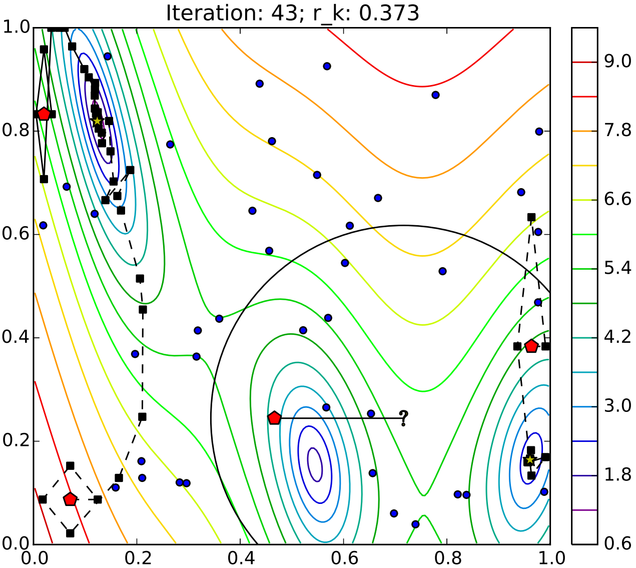
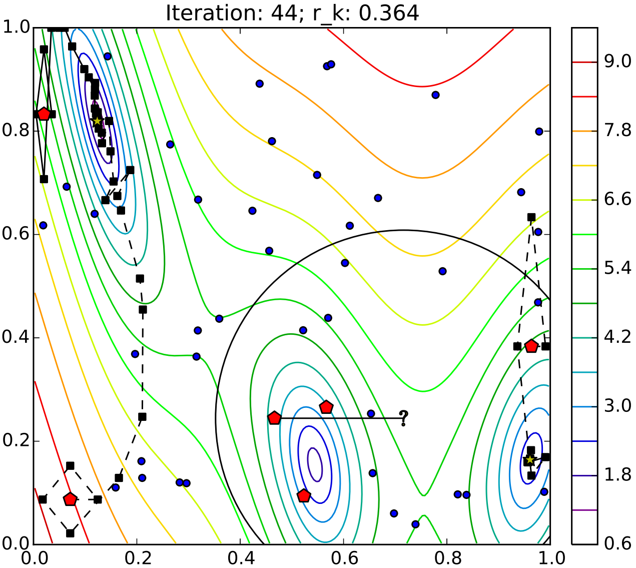


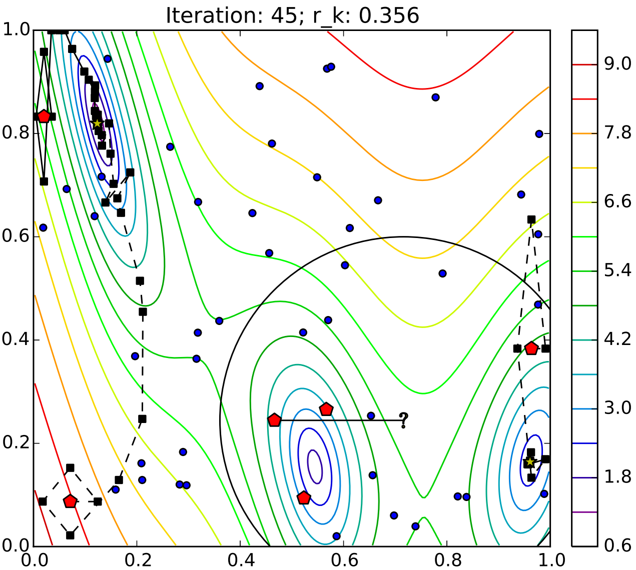
Pausing runs



Pausing runs



Pausing runs



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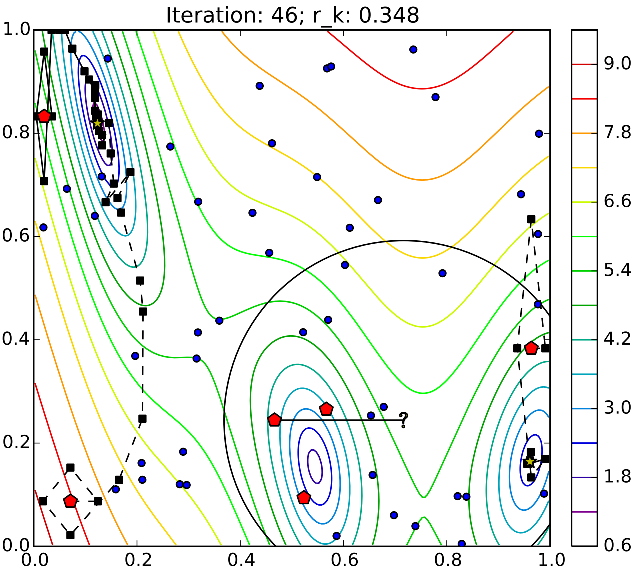

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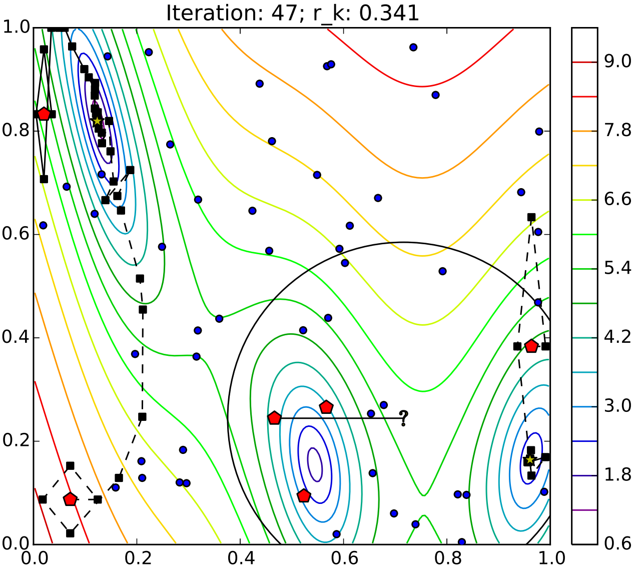

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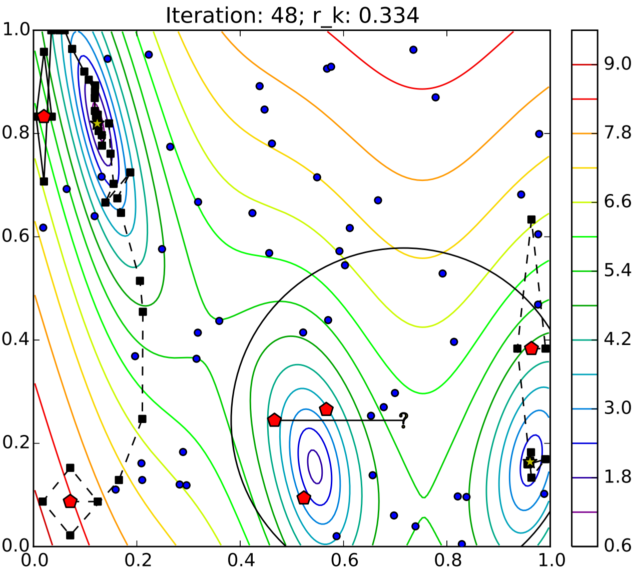

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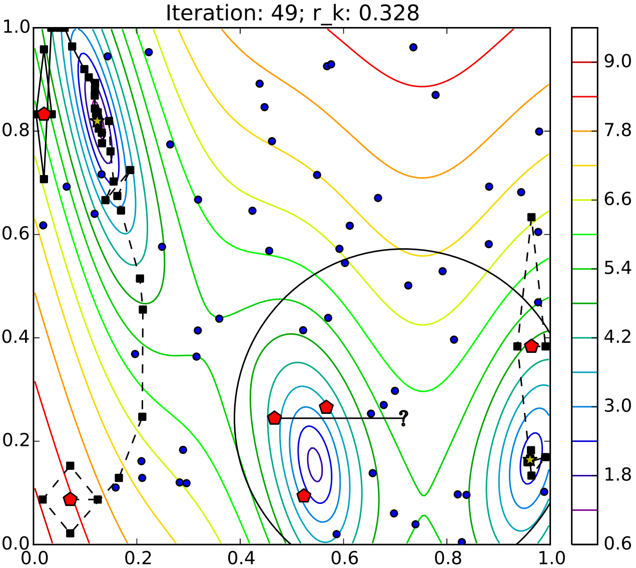

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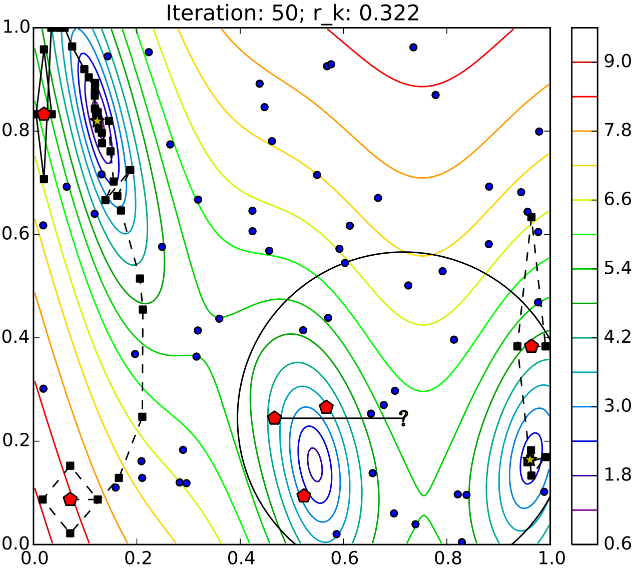

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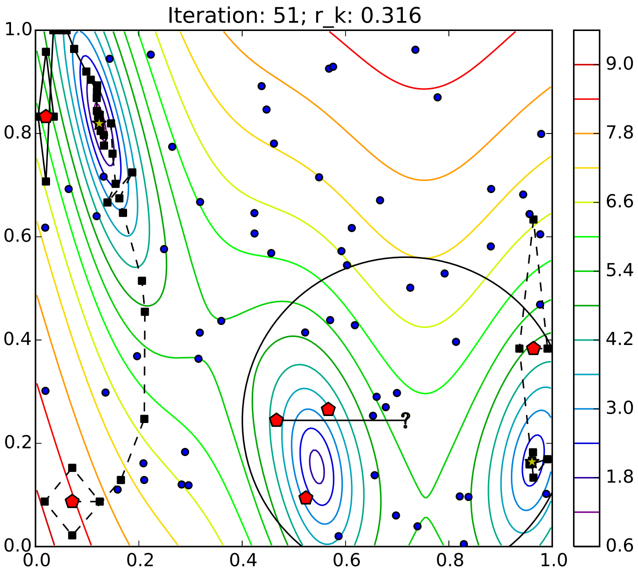

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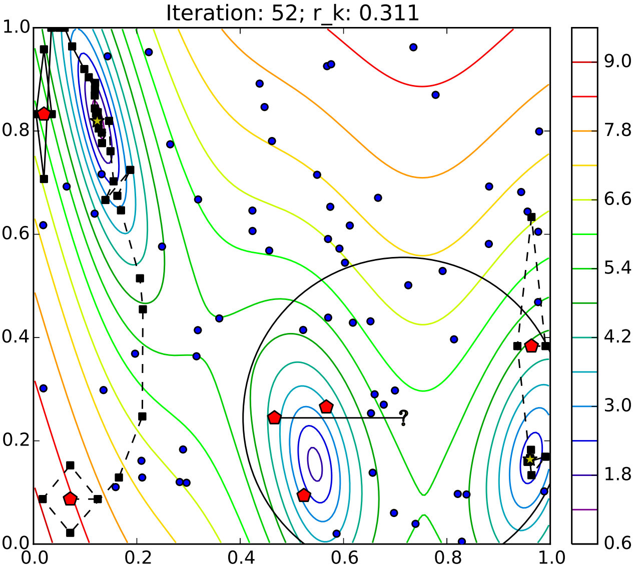

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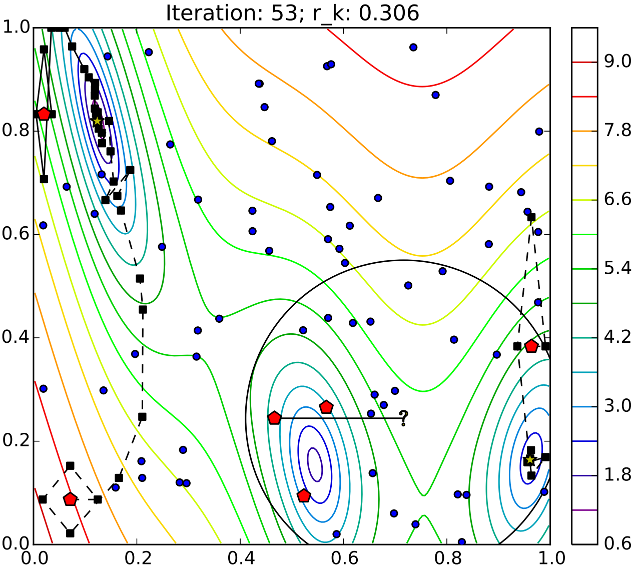

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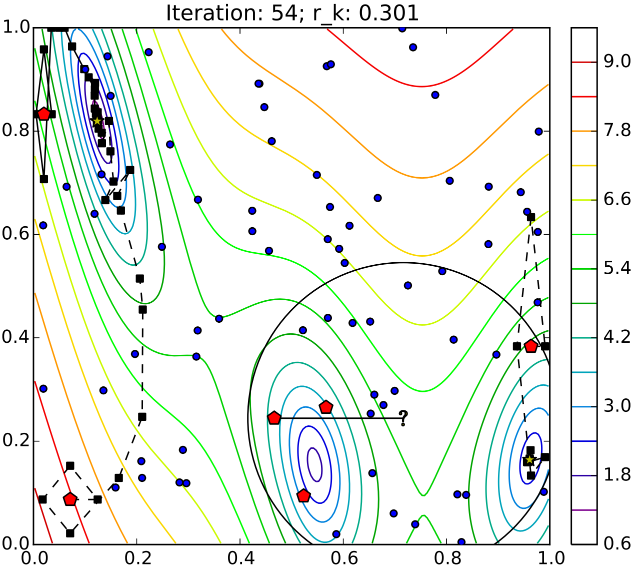

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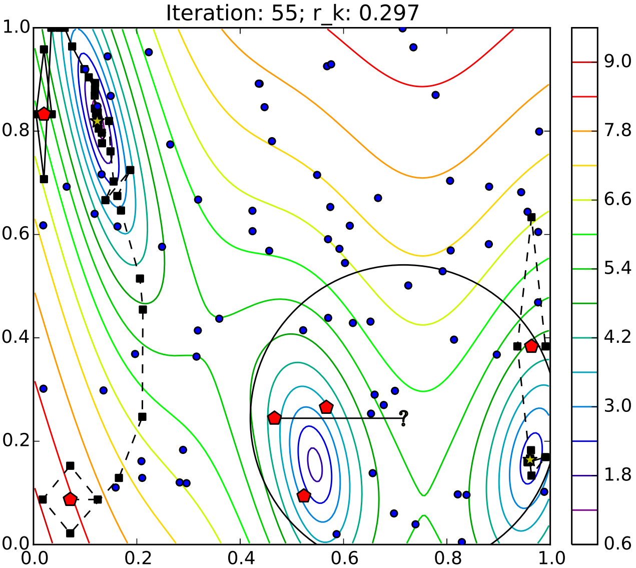

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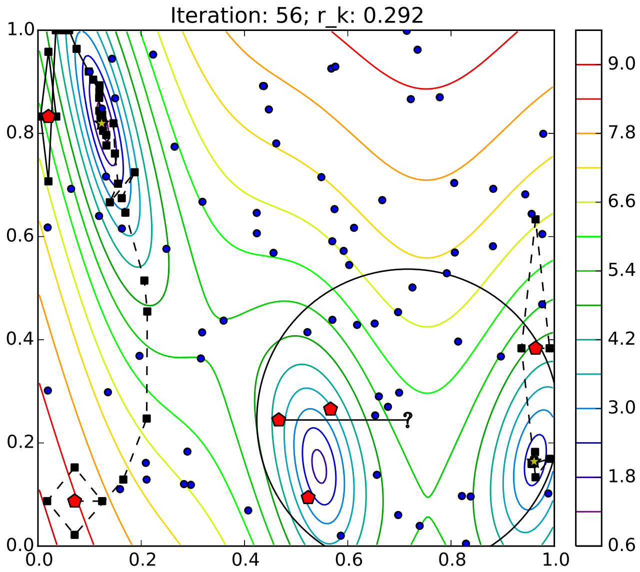

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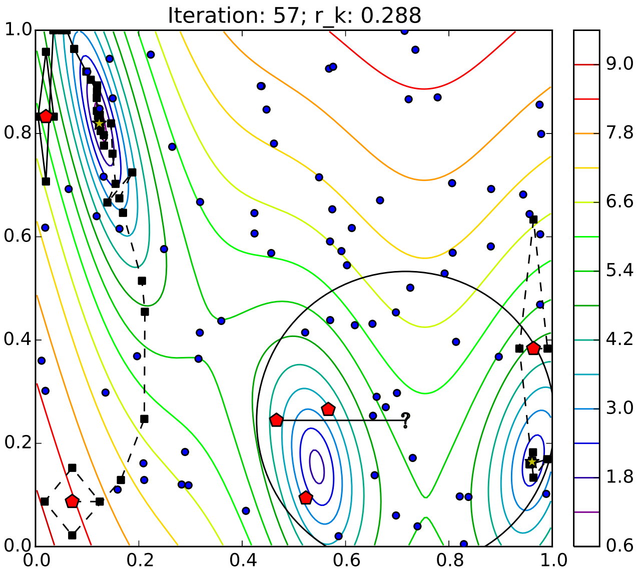

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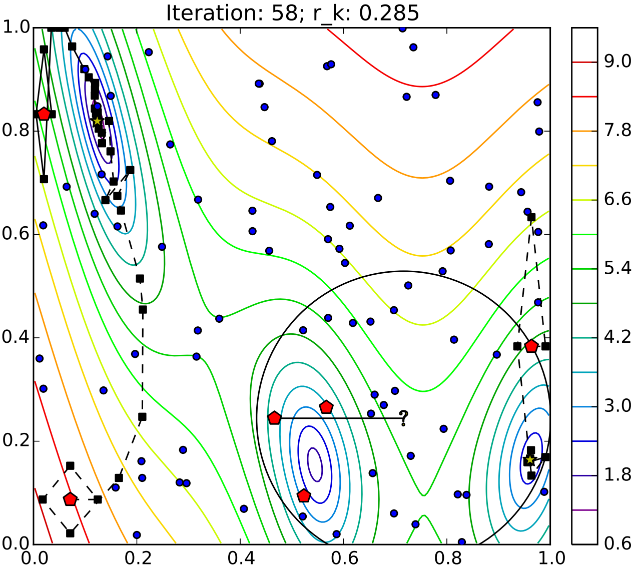

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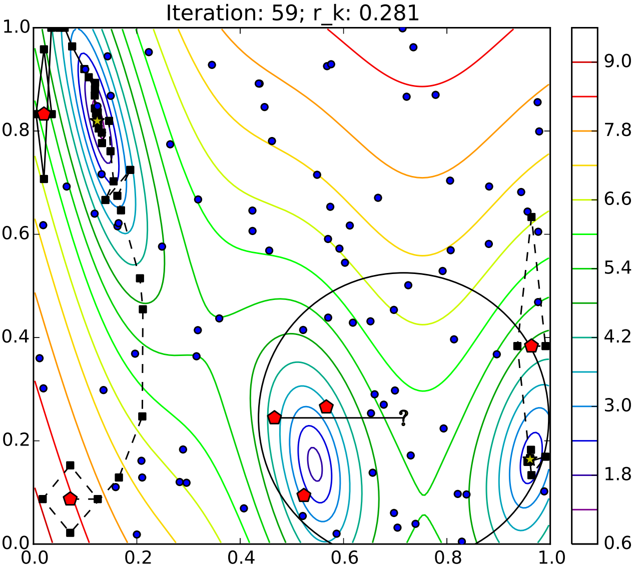

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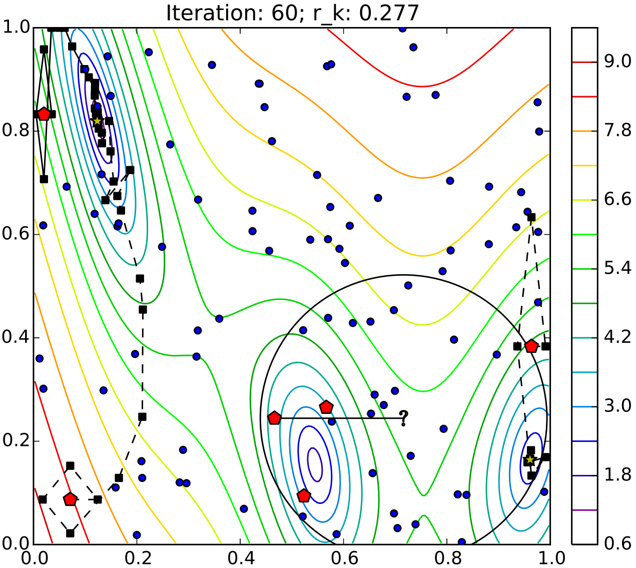

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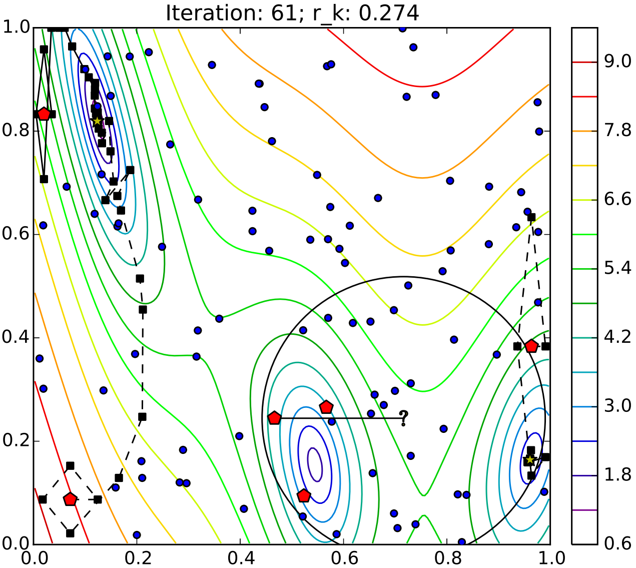

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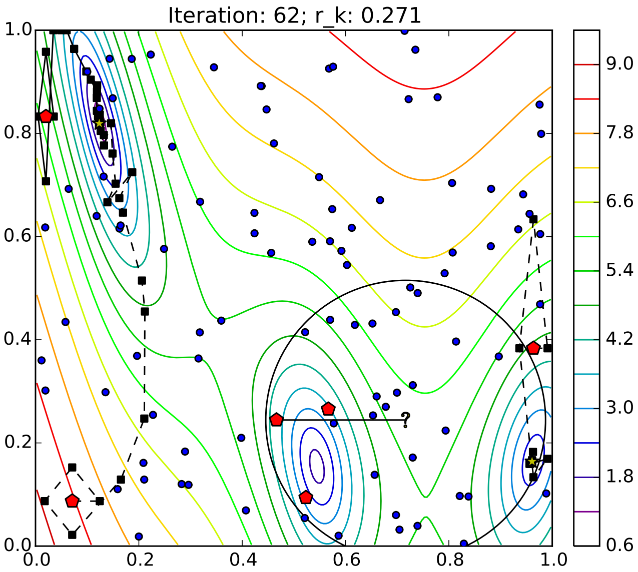

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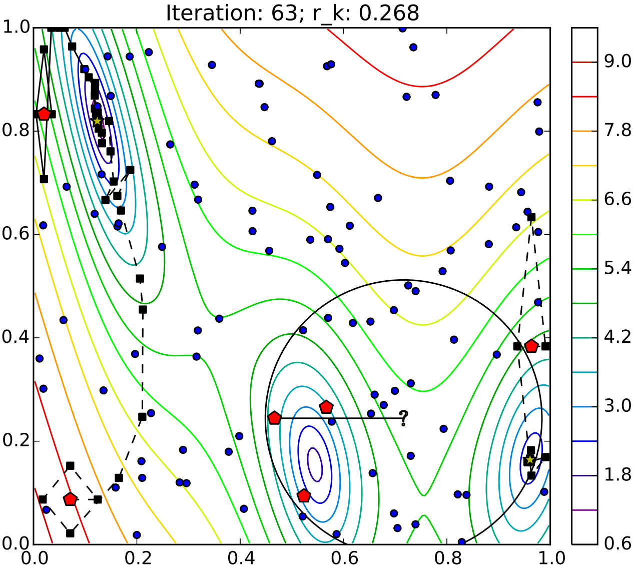

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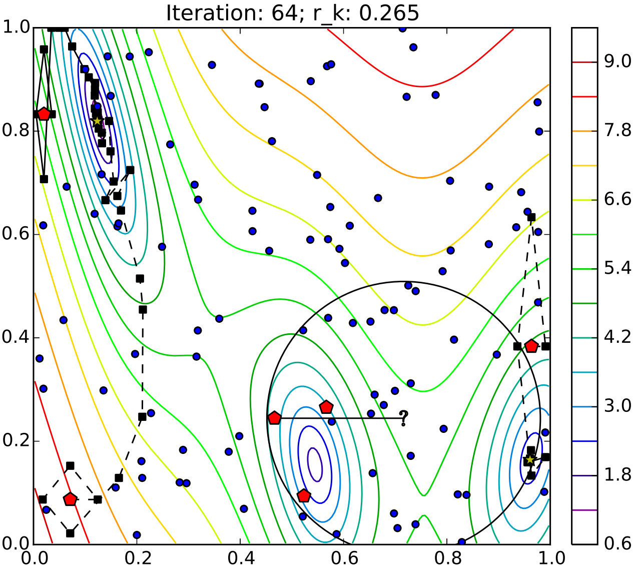

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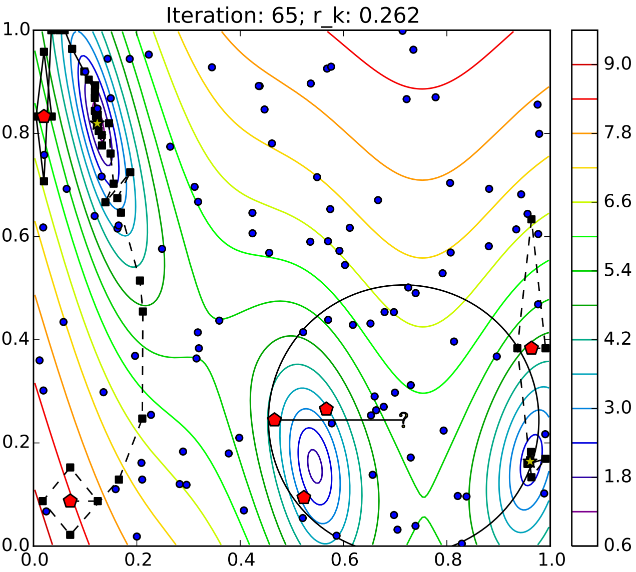

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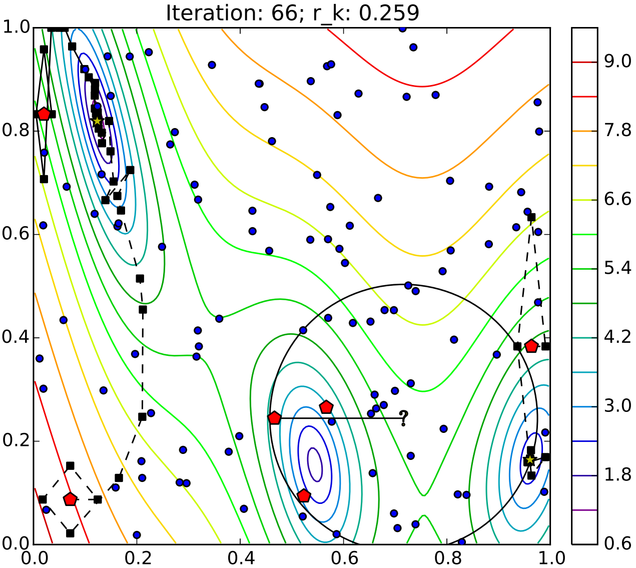

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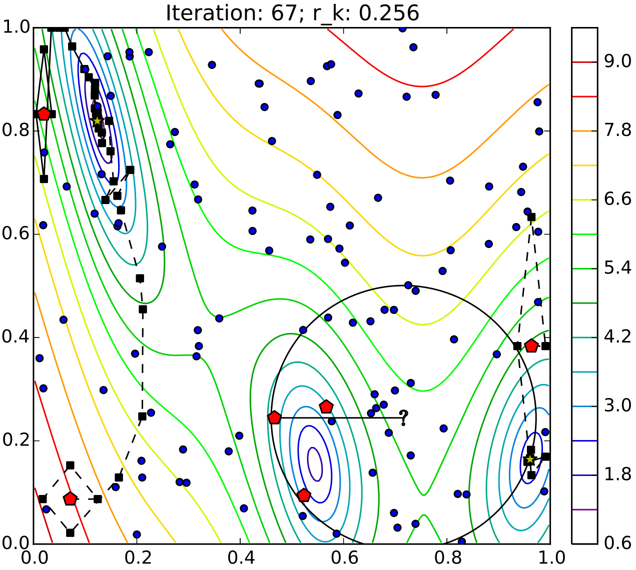

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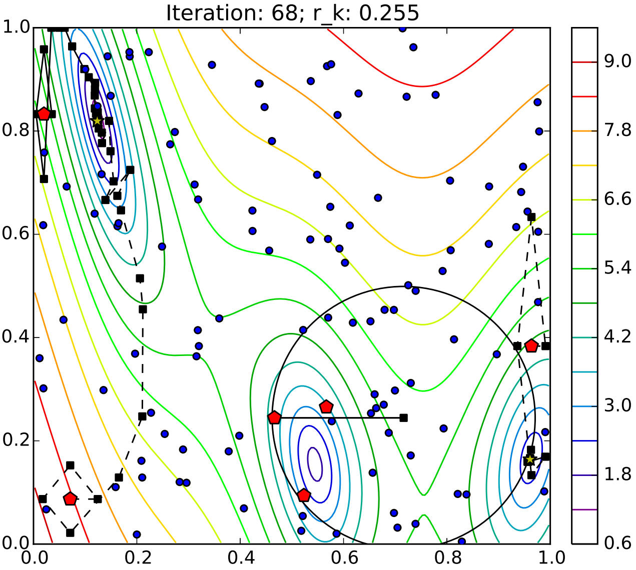

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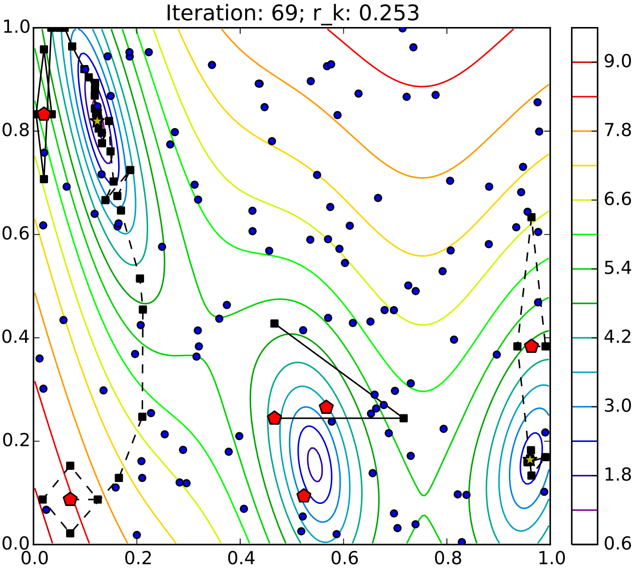

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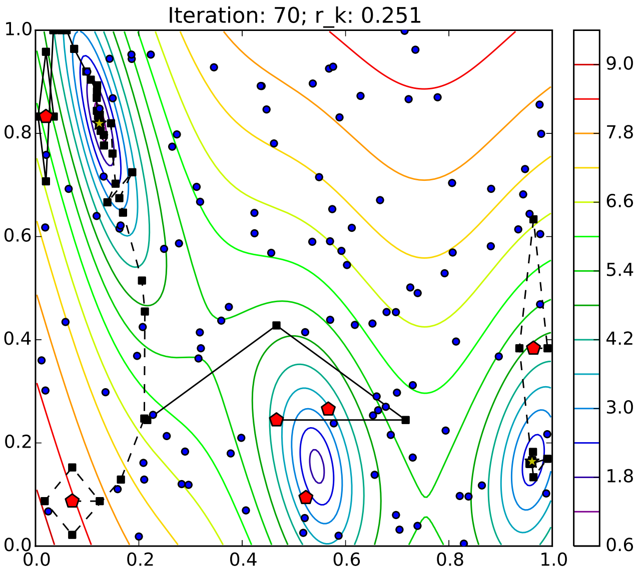

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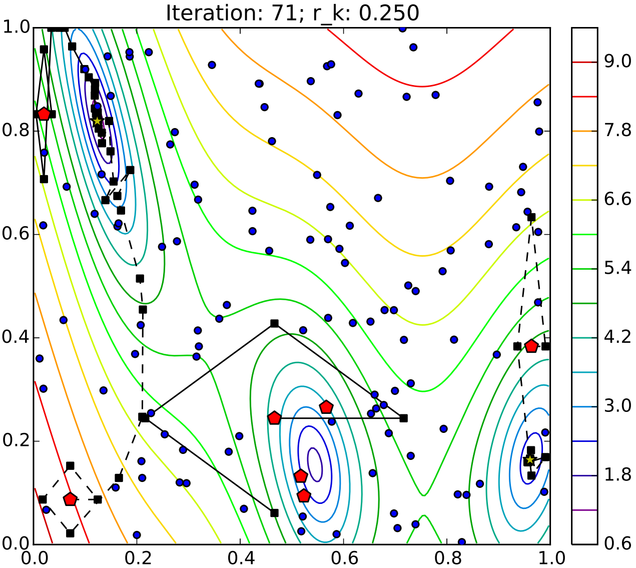

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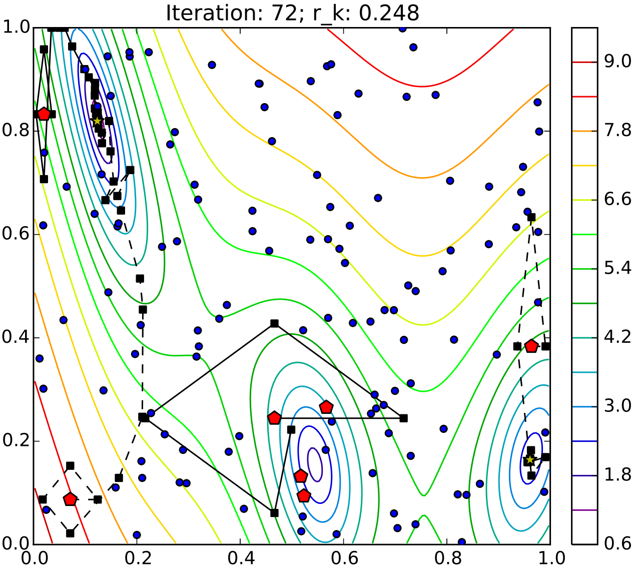

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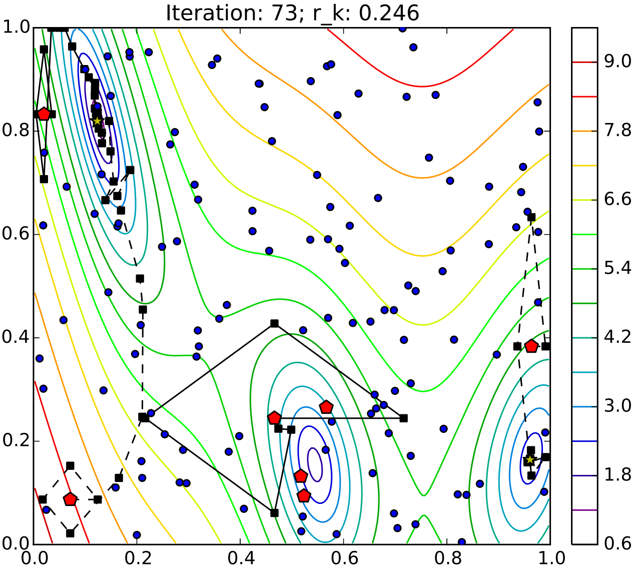

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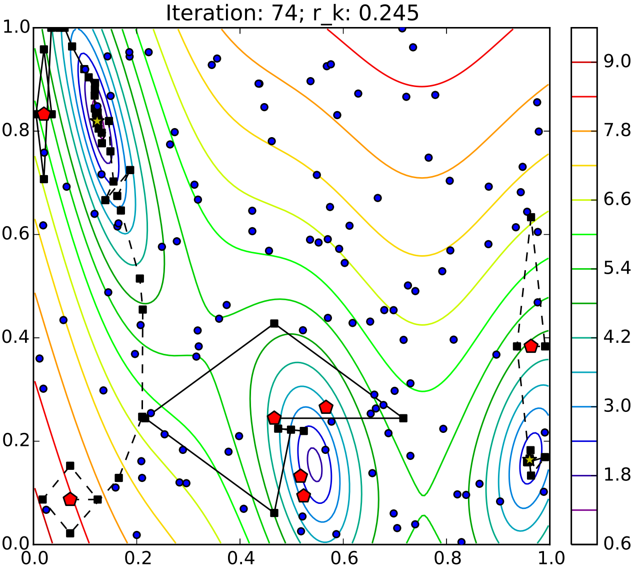

Pausing runs